



# Full wwPDB Geometry-Only Validation Report ⓘ

Mar 11, 2018 – 04:22 pm GMT

PDB ID : 3B5U  
Title : Actin filament model from extended form of acromsomal bundle in the Limulus sperm  
Authors : Cong, Y.; Topf, M.; Sali, A.; Matsudaira, P.; Dougherty, M.; Chiu, W.; Schmid, M.F.  
Deposited on : 2007-10-26  
Resolution : 9.50 Å(reported)

This is a Full wwPDB Geometry-Only Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

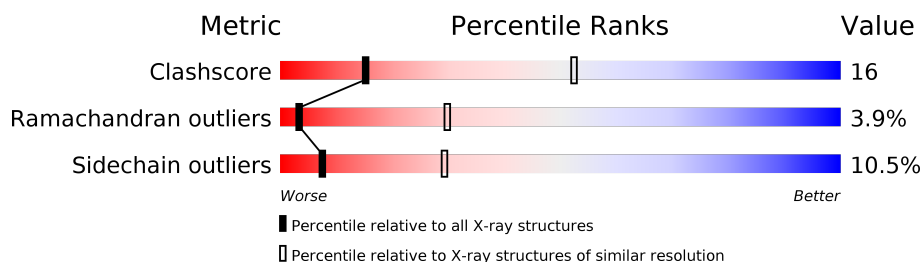
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON CRYSTALLOGRAPHY*

The reported resolution of this entry is 9.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122126	1148 (15.00-3.80)
Ramachandran outliers	120053	1072 (11.50-3.80)
Sidechain outliers	120020	1039 (11.50-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	377	57% 36% 5% ..
1	B	377	58% 34% 6% ..
1	C	377	66% 27% 6% .
1	D	377	57% 33% 9% ..
1	E	377	60% 29% 9% ..
1	F	377	58% 34% 6% ..
1	G	377	65% 29% 6% .
1	H	377	69% 27% . ..

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Mol	Chain	Length	Quality of chain
1	I	377	<div><div></div><div>61%33%6%..</div></div>
1	J	377	<div><div></div><div>60%31%6%..</div></div>
1	K	377	<div><div></div><div>61%31%6%..</div></div>
1	L	377	<div><div></div><div>56%36%6%..</div></div>
1	M	377	<div><div></div><div>64%28%6%..</div></div>
1	N	377	<div><div></div><div>57%32%9%..</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 41062 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Actin, alpha skeletal muscle.

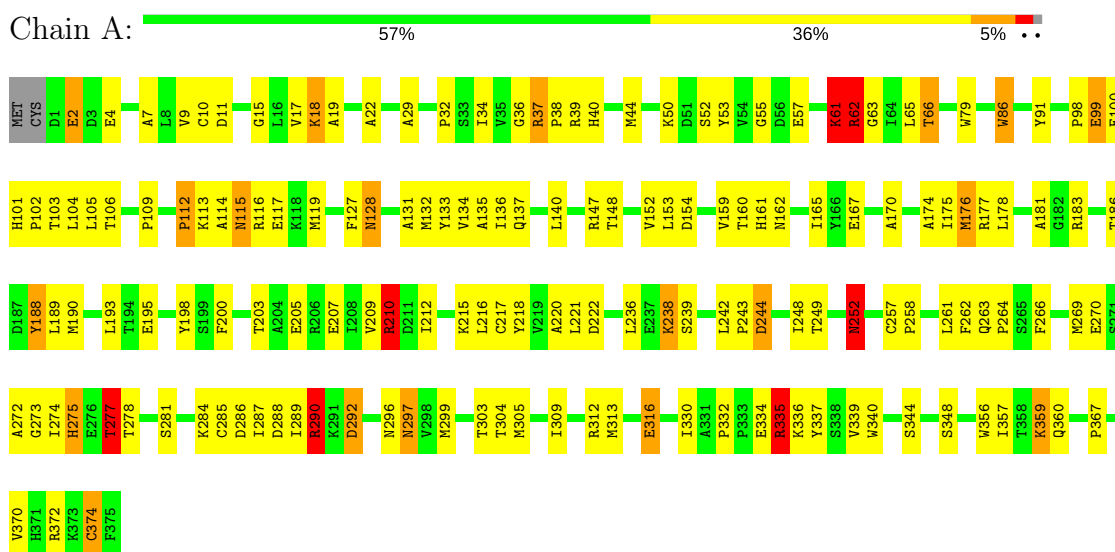
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	B	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	C	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	D	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	E	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	F	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	G	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	H	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	I	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	J	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	K	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	L	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	M	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			
1	N	375	Total	C	N	O	S	0	0	0
			2933	1854	493	565	21			

### 3 Residue-property plots

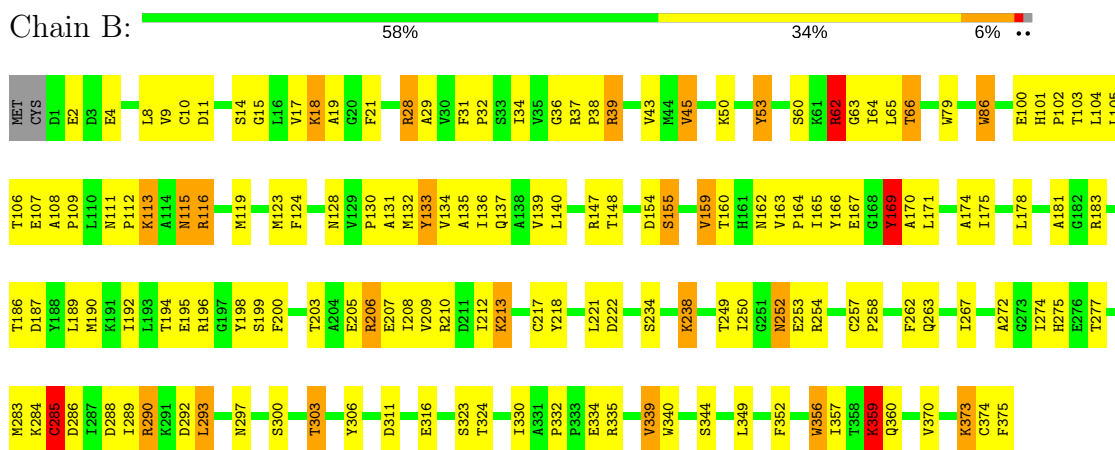
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: Actin, alpha skeletal muscle

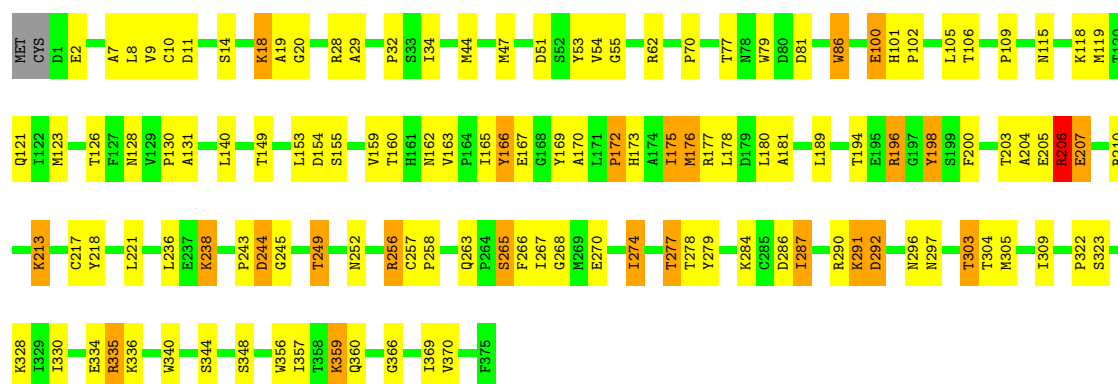


- Molecule 1: Actin, alpha skeletal muscle

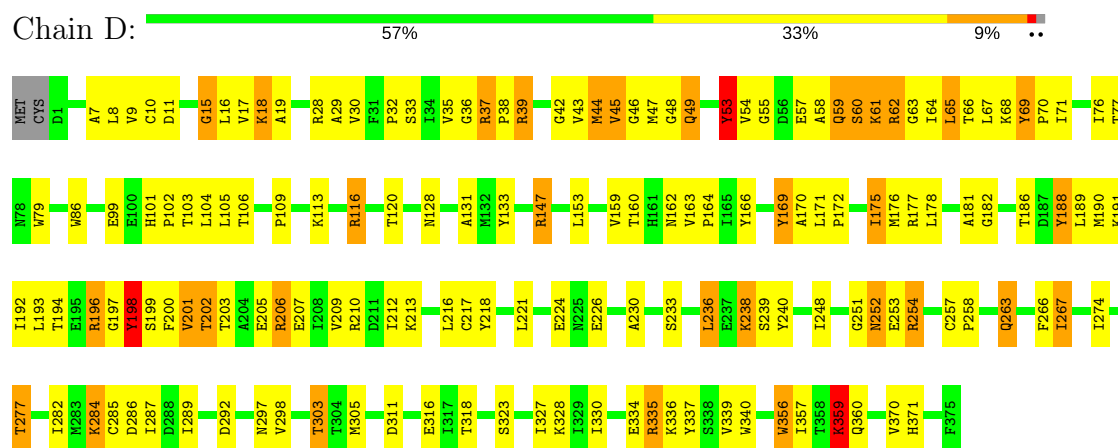


- Molecule 1: Actin, alpha skeletal muscle

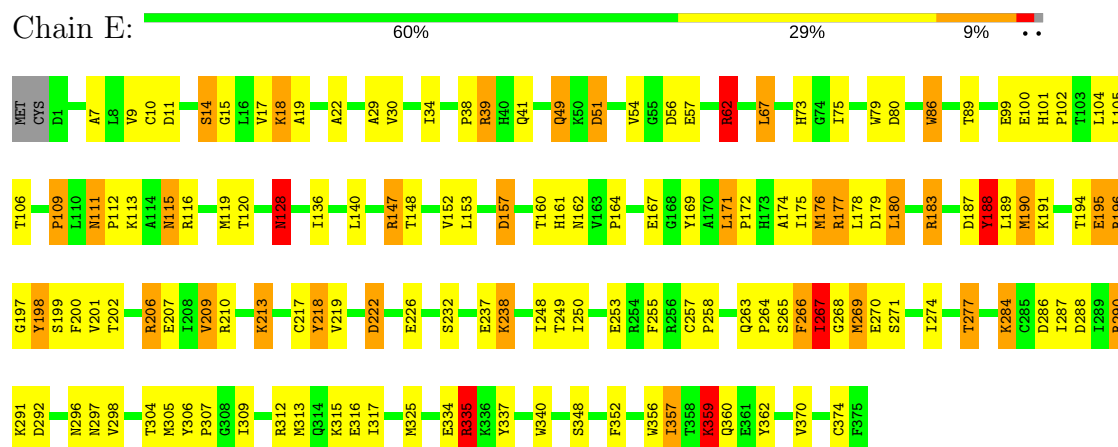




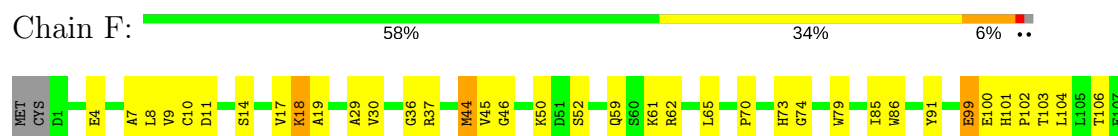
- Molecule 1: Actin, alpha skeletal muscle



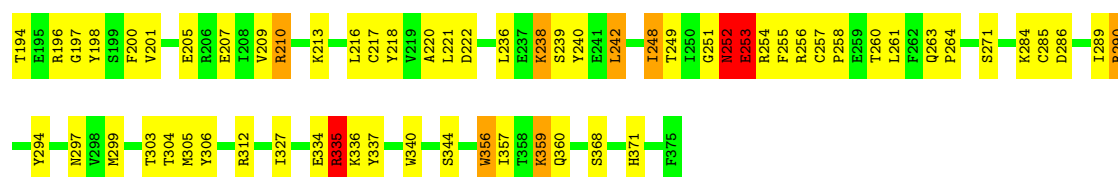
- Molecule 1: Actin, alpha skeletal muscle



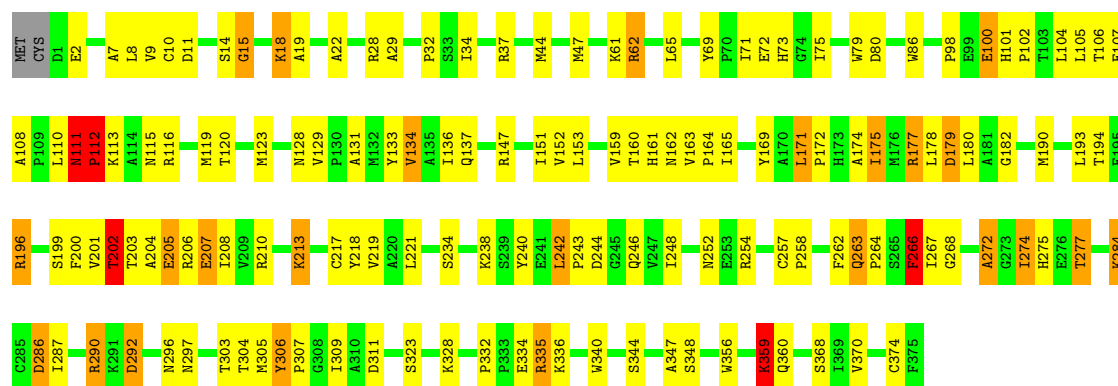
- Molecule 1: Actin, alpha skeletal muscle



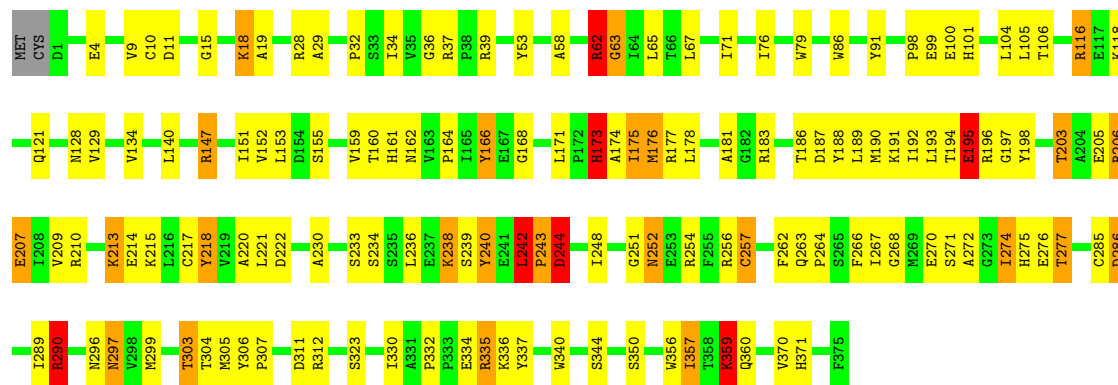




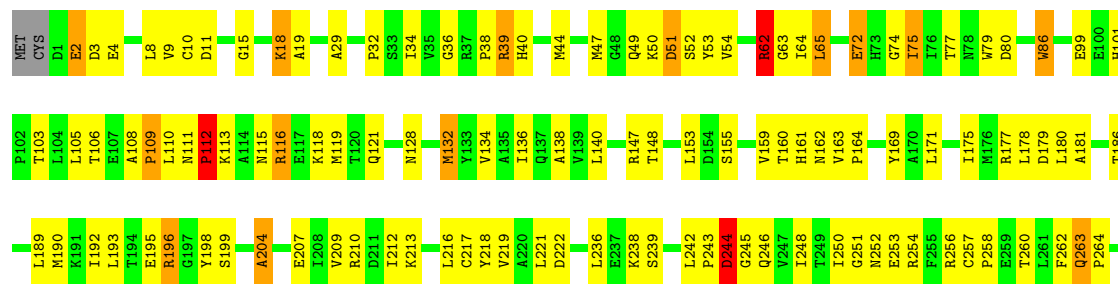
• Molecule 1: Actin, alpha skeletal muscle



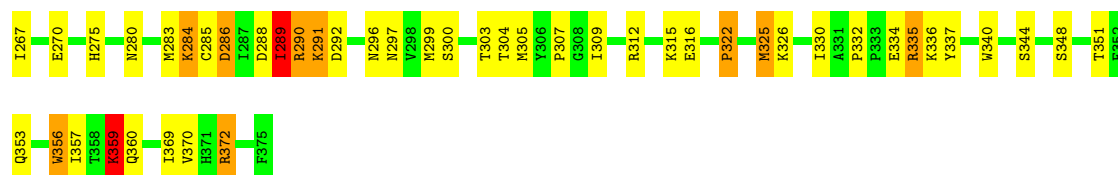
• Molecule 1: Actin, alpha skeletal muscle



• Molecule 1: Actin, alpha skeletal muscle

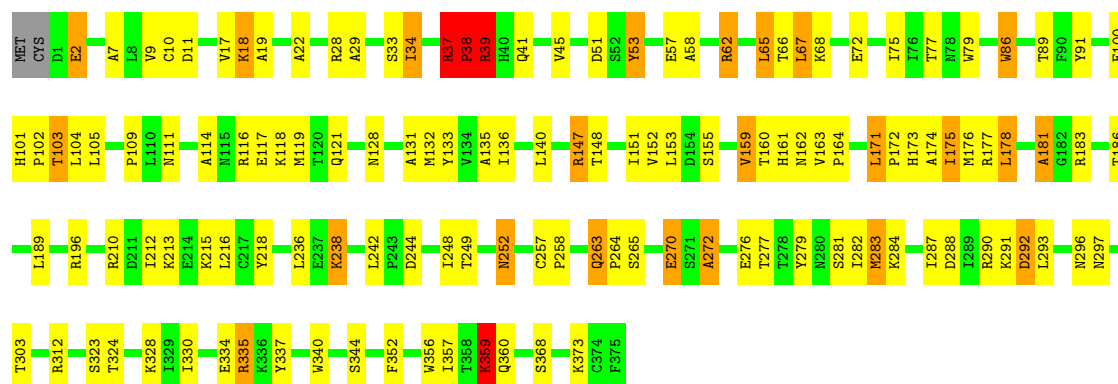






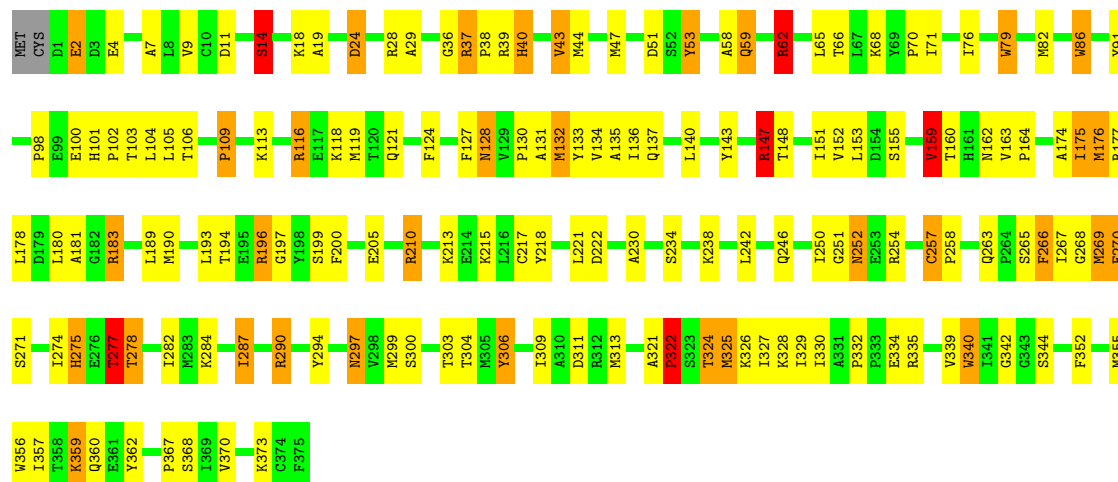
- Molecule 1: Actin, alpha skeletal muscle

Chain M: 64% 28% 6% ..



- Molecule 1: Actin, alpha skeletal muscle

Chain N: 57% 32% 9% ..



## 4 Model quality

### 4.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.69	0/2996	1.34	21/4058 (0.5%)
1	B	0.68	0/2996	1.35	23/4058 (0.6%)
1	C	0.64	0/2996	1.30	22/4058 (0.5%)
1	D	0.66	0/2996	1.42	33/4058 (0.8%)
1	E	0.65	0/2996	1.40	30/4058 (0.7%)
1	F	0.64	0/2996	1.34	19/4058 (0.5%)
1	G	0.65	0/2996	1.29	23/4058 (0.6%)
1	H	0.67	0/2996	1.32	20/4058 (0.5%)
1	I	0.67	0/2996	1.29	24/4058 (0.6%)
1	J	1.60	6/2996 (0.2%)	1.32	22/4058 (0.5%)
1	K	2.88	3/2996 (0.1%)	1.40	36/4058 (0.9%)
1	L	1.19	5/2996 (0.2%)	1.39	28/4058 (0.7%)
1	M	0.69	0/2996	1.40	27/4058 (0.7%)
1	N	0.69	0/2996	1.39	32/4058 (0.8%)
All	All	1.11	14/41944 (0.0%)	1.35	360/56812 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	11
1	C	0	7
1	D	0	11
1	E	0	10
1	F	0	8
1	G	0	3
1	H	0	6
1	I	0	9
1	J	0	8
1	K	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	13
1	M	0	7
1	N	0	10
All	All	0	123

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	195	GLU	CB-CG	122.37	3.84	1.52
1	K	173	HIS	CB-CG	91.74	3.15	1.50
1	J	266	PHE	CG-CD2	38.22	1.96	1.38
1	J	266	PHE	CG-CD1	37.55	1.95	1.38
1	J	266	PHE	CE2-CZ	30.64	1.95	1.37
1	J	266	PHE	CE1-CZ	30.50	1.95	1.37
1	L	112	PRO	CA-CB	30.17	2.13	1.53
1	L	112	PRO	N-CD	28.91	1.88	1.47
1	J	266	PHE	CD2-CE2	28.12	1.95	1.39
1	J	266	PHE	CD1-CE1	27.36	1.94	1.39
1	L	112	PRO	CG-CD	21.76	2.22	1.50
1	L	112	PRO	N-CA	21.55	1.83	1.47
1	L	112	PRO	CB-CG	12.60	2.12	1.50
1	K	173	HIS	CG-CD2	5.44	1.45	1.35

All (360) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	173	HIS	CA-CB-CG	16.70	141.98	113.60
1	E	177	ARG	NE-CZ-NH2	11.76	126.18	120.30
1	M	183	ARG	NE-CZ-NH2	-11.55	114.53	120.30
1	D	116	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	N	196	ARG	NE-CZ-NH2	-10.23	115.19	120.30
1	E	39	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	E	196	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	L	112	PRO	CA-N-CD	9.58	125.11	111.70
1	K	195	GLU	CA-CB-CG	9.45	134.18	113.40
1	B	356	TRP	CD1-CG-CD2	9.32	113.76	106.30
1	K	173	HIS	ND1-CG-CD2	-9.22	93.09	106.00
1	M	39	ARG	NE-CZ-NH1	-9.10	115.75	120.30
1	M	79	TRP	CD1-CG-CD2	9.09	113.58	106.30
1	H	116	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	E	196	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	E	39	ARG	NE-CZ-NH2	-9.04	115.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	28	ARG	NE-CZ-NH1	-8.95	115.83	120.30
1	N	116	ARG	NE-CZ-NH2	8.89	124.74	120.30
1	K	79	TRP	CD1-CG-CD2	8.83	113.36	106.30
1	A	356	TRP	CD1-CG-CD2	8.78	113.32	106.30
1	K	28	ARG	NE-CZ-NH1	-8.76	115.92	120.30
1	B	356	TRP	CE2-CD2-CG	-8.71	100.34	107.30
1	E	177	ARG	NE-CZ-NH1	-8.64	115.98	120.30
1	L	79	TRP	CD1-CG-CD2	8.56	113.15	106.30
1	H	356	TRP	CD1-CG-CD2	8.52	113.12	106.30
1	M	86	TRP	CD1-CG-CD2	8.52	113.11	106.30
1	H	86	TRP	CD1-CG-CD2	8.51	113.11	106.30
1	D	356	TRP	CD1-CG-CD2	8.50	113.10	106.30
1	C	356	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	E	86	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	H	356	TRP	CE2-CD2-CG	-8.45	100.54	107.30
1	N	79	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	B	79	TRP	CD1-CG-CD2	8.43	113.05	106.30
1	E	79	TRP	CD1-CG-CD2	8.42	113.03	106.30
1	M	79	TRP	CE2-CD2-CG	-8.42	100.57	107.30
1	N	79	TRP	CE2-CD2-CG	-8.40	100.58	107.30
1	D	177	ARG	NE-CZ-NH1	-8.40	116.10	120.30
1	C	79	TRP	CD1-CG-CD2	8.40	113.02	106.30
1	H	79	TRP	CD1-CG-CD2	8.40	113.02	106.30
1	F	356	TRP	CD1-CG-CD2	8.31	112.95	106.30
1	J	79	TRP	CD1-CG-CD2	8.30	112.94	106.30
1	J	356	TRP	CD1-CG-CD2	8.29	112.93	106.30
1	M	37	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	K	86	TRP	CD1-CG-CD2	8.27	112.92	106.30
1	D	356	TRP	CE2-CD2-CG	-8.25	100.70	107.30
1	N	356	TRP	CD1-CG-CD2	8.24	112.89	106.30
1	C	86	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	K	356	TRP	CD1-CG-CD2	8.22	112.87	106.30
1	G	335	ARG	NE-CZ-NH1	-8.21	116.19	120.30
1	G	86	TRP	CD1-CG-CD2	8.21	112.86	106.30
1	G	356	TRP	CD1-CG-CD2	8.18	112.85	106.30
1	J	86	TRP	CD1-CG-CD2	8.18	112.85	106.30
1	A	79	TRP	CD1-CG-CD2	8.17	112.84	106.30
1	B	79	TRP	CE2-CD2-CG	-8.14	100.79	107.30
1	K	340	TRP	CD1-CG-CD2	8.11	112.79	106.30
1	I	79	TRP	CD1-CG-CD2	8.11	112.79	106.30
1	L	356	TRP	CE2-CD2-CG	-8.11	100.81	107.30
1	M	356	TRP	CD1-CG-CD2	8.09	112.77	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	340	TRP	CD1-CG-CD2	8.08	112.76	106.30
1	F	86	TRP	CD1-CG-CD2	8.07	112.75	106.30
1	E	356	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	N	340	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	M	28	ARG	NE-CZ-NH1	-8.04	116.28	120.30
1	I	356	TRP	CD1-CG-CD2	8.03	112.73	106.30
1	A	356	TRP	CE2-CD2-CG	-8.03	100.88	107.30
1	H	79	TRP	CE2-CD2-CG	-8.00	100.90	107.30
1	G	356	TRP	CE2-CD2-CG	-8.00	100.90	107.30
1	A	340	TRP	CD1-CG-CD2	7.99	112.69	106.30
1	K	39	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	A	79	TRP	CE2-CD2-CG	-7.93	100.96	107.30
1	C	356	TRP	CE2-CD2-CG	-7.92	100.97	107.30
1	F	177	ARG	NE-CZ-NH1	-7.89	116.36	120.30
1	M	356	TRP	CE2-CD2-CG	-7.89	100.99	107.30
1	L	356	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	D	340	TRP	CD1-CG-CD2	7.87	112.60	106.30
1	G	79	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	E	356	TRP	CE2-CD2-CG	-7.83	101.04	107.30
1	K	177	ARG	NE-CZ-NH1	-7.82	116.39	120.30
1	E	79	TRP	CE2-CD2-CG	-7.82	101.05	107.30
1	G	340	TRP	CD1-CG-CD2	7.82	112.55	106.30
1	L	86	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	M	340	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	H	340	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	H	86	TRP	CE2-CD2-CG	-7.77	101.08	107.30
1	J	340	TRP	CE2-CD2-CG	-7.76	101.09	107.30
1	J	86	TRP	CE2-CD2-CG	-7.75	101.10	107.30
1	F	79	TRP	CD1-CG-CD2	7.72	112.48	106.30
1	H	340	TRP	CE2-CD2-CG	-7.72	101.12	107.30
1	J	340	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	B	28	ARG	NE-CZ-NH1	-7.70	116.45	120.30
1	K	79	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	J	356	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	C	79	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	B	340	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	I	340	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	B	340	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	E	86	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	D	86	TRP	CD1-CG-CD2	7.66	112.42	106.30
1	G	79	TRP	CE2-CD2-CG	-7.66	101.18	107.30
1	F	356	TRP	CE2-CD2-CG	-7.65	101.18	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	79	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	D	340	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	L	112	PRO	N-CA-C	7.59	131.83	112.10
1	L	79	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	B	86	TRP	CD1-CG-CD2	7.55	112.34	106.30
1	J	79	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	C	340	TRP	CD1-CG-CD2	7.54	112.33	106.30
1	K	356	TRP	CE2-CD2-CG	-7.53	101.27	107.30
1	I	340	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	C	86	TRP	CE2-CD2-CG	-7.48	101.31	107.30
1	L	340	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	N	340	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	E	218	TYR	CB-CG-CD1	-7.46	116.53	121.00
1	K	86	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	M	340	TRP	CE2-CD2-CG	-7.43	101.35	107.30
1	K	340	TRP	CE2-CD2-CG	-7.43	101.36	107.30
1	L	340	TRP	CD1-CG-CD2	7.43	112.24	106.30
1	A	340	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	L	72	GLU	CA-C-N	-7.41	100.91	117.20
1	I	356	TRP	CE2-CD2-CG	-7.39	101.39	107.30
1	E	340	TRP	CE2-CD2-CG	-7.39	101.39	107.30
1	C	335	ARG	NE-CZ-NH1	-7.38	116.61	120.30
1	G	86	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	C	340	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	A	86	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	G	340	TRP	CE2-CD2-CG	-7.28	101.47	107.30
1	D	254	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	K	183	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	L	62	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	F	86	TRP	CE2-CD2-CG	-7.26	101.49	107.30
1	D	86	TRP	CE2-CD2-CG	-7.23	101.52	107.30
1	I	79	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	N	86	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	M	86	TRP	CE2-CD2-CG	-7.18	101.56	107.30
1	D	147	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	D	79	TRP	CE2-CD2-CG	-7.14	101.58	107.30
1	D	79	TRP	CD1-CG-CD2	7.14	112.01	106.30
1	I	86	TRP	CD1-CG-CD2	7.14	112.02	106.30
1	F	116	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	D	206	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	H	356	TRP	CG-CD2-CE3	7.05	140.25	133.90
1	G	62	ARG	NE-CZ-NH2	7.05	123.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	356	TRP	CE2-CD2-CG	-7.03	101.67	107.30
1	N	39	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	L	112	PRO	CA-C-N	-7.02	101.75	117.20
1	L	86	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	B	86	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	H	356	TRP	CB-CG-CD1	-6.95	117.96	127.00
1	N	86	TRP	CE2-CD2-CG	-6.91	101.77	107.30
1	A	290	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	N	28	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	A	183	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	K	173	HIS	CG-ND1-CE1	6.85	117.78	108.20
1	J	177	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	D	69	TYR	CB-CG-CD2	-6.80	116.92	121.00
1	M	335	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	K	116	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	H	177	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	F	340	TRP	CE2-CD2-CG	-6.72	101.92	107.30
1	F	196	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	E	335	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	E	188	TYR	CB-CG-CD2	-6.69	116.98	121.00
1	F	340	TRP	CD1-CG-CD2	6.69	111.66	106.30
1	L	244	ASP	CA-C-N	6.68	129.56	116.20
1	I	290	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	N	277	THR	CA-CB-CG2	6.65	121.70	112.40
1	A	62	ARG	O-C-N	-6.64	111.91	123.20
1	K	195	GLU	CB-CG-CD	6.60	132.01	114.20
1	H	277	THR	N-CA-CB	-6.59	97.77	110.30
1	B	356	TRP	CG-CD2-CE3	6.56	139.80	133.90
1	B	356	TRP	CB-CG-CD1	-6.55	118.49	127.00
1	N	322	PRO	CA-N-CD	-6.54	102.35	111.50
1	J	356	TRP	CG-CD2-CE3	6.52	139.77	133.90
1	K	218	TYR	CB-CG-CD1	-6.52	117.09	121.00
1	B	39	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	D	335	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	D	28	ARG	NE-CZ-NH1	-6.49	117.06	120.30
1	E	183	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	B	169	TYR	CB-CG-CD2	-6.46	117.12	121.00
1	L	290	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	N	183	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	335	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	N	322	PRO	N-CA-C	6.42	128.80	112.10
1	E	206	ARG	NE-CZ-NH1	6.41	123.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	335	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	I	86	TRP	CE2-CD2-CG	-6.38	102.20	107.30
1	D	356	TRP	CB-CG-CD1	-6.34	118.76	127.00
1	C	177	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	A	62	ARG	CA-C-N	6.32	128.84	116.20
1	A	86	TRP	CE2-CD2-CG	-6.30	102.26	107.30
1	L	244	ASP	O-C-N	-6.30	112.49	123.20
1	B	196	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	D	356	TRP	CG-CD2-CE3	6.26	139.54	133.90
1	D	39	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	C	28	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	I	356	TRP	CB-CG-CD1	-6.21	118.93	127.00
1	J	177	ARG	NE-CZ-NH2	6.21	123.40	120.30
1	M	37	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	G	356	TRP	CB-CG-CD1	-6.13	119.03	127.00
1	C	28	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	L	356	TRP	CG-CD2-CE3	6.10	139.39	133.90
1	L	147	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	277	THR	CA-CB-CG2	6.09	120.93	112.40
1	D	198	TYR	CA-C-N	6.07	130.56	117.20
1	N	79	TRP	CG-CD2-CE3	6.07	139.36	133.90
1	G	356	TRP	CG-CD2-CE3	6.07	139.36	133.90
1	K	290	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	M	196	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	H	277	THR	CA-CB-CG2	6.04	120.86	112.40
1	D	202	THR	N-CA-CB	6.03	121.76	110.30
1	J	28	ARG	NE-CZ-NH1	-6.01	117.29	120.30
1	K	206	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	B	79	TRP	CG-CD2-CE3	6.00	139.30	133.90
1	I	147	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	356	TRP	CG-CD1-NE1	-5.97	104.13	110.10
1	D	218	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	N	290	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	B	290	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	K	303	THR	CA-CB-CG2	5.93	120.71	112.40
1	M	177	ARG	NE-CZ-NH1	-5.91	117.35	120.30
1	D	188	TYR	CB-CG-CD2	-5.91	117.46	121.00
1	I	356	TRP	CG-CD2-CE3	5.90	139.21	133.90
1	C	356	TRP	CG-CD2-CE3	5.87	139.19	133.90
1	G	155	SER	CA-C-N	-5.85	104.50	116.20
1	J	277	THR	CA-CB-CG2	5.85	120.59	112.40
1	G	290	ARG	NE-CZ-NH2	-5.83	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	303	THR	CA-CB-CG2	5.81	120.53	112.40
1	B	196	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	F	285	CYS	C-N-CA	5.79	136.16	121.70
1	N	147	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	K	244	ASP	N-CA-CB	-5.78	100.19	110.60
1	F	335	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	K	356	TRP	CB-CG-CD1	-5.75	119.53	127.00
1	M	79	TRP	CG-CD2-CE3	5.74	139.07	133.90
1	G	177	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	J	356	TRP	CB-CG-CD1	-5.74	119.54	127.00
1	N	278	THR	CA-CB-CG2	5.73	120.42	112.40
1	D	198	TYR	O-C-N	-5.72	113.54	122.70
1	E	356	TRP	CG-CD2-CE3	5.72	139.05	133.90
1	M	116	ARG	NE-CZ-NH2	5.71	123.16	120.30
1	I	196	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	M	356	TRP	CG-CD2-CE3	5.70	139.03	133.90
1	A	292	ASP	CB-CG-OD1	5.69	123.42	118.30
1	H	303	THR	CA-CB-CG2	5.68	120.36	112.40
1	B	183	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	C	206	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	177	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	N	177	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	I	306	TYR	CB-CG-CD2	-5.62	117.62	121.00
1	B	303	THR	CA-CB-CG2	5.62	120.27	112.40
1	G	120	THR	CA-CB-OG1	-5.62	97.20	109.00
1	C	196	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	K	242	LEU	CA-CB-CG	5.61	128.20	115.30
1	L	116	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	F	265	SER	N-CA-CB	5.60	118.90	110.50
1	N	53	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	N	177	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	L	196	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	H	79	TRP	CG-CD2-CE3	5.55	138.89	133.90
1	K	79	TRP	CG-CD1-NE1	-5.53	104.58	110.10
1	E	267	ILE	CA-C-N	5.52	127.25	116.20
1	J	340	TRP	CG-CD2-CE3	5.51	138.86	133.90
1	K	177	ARG	NE-CZ-NH2	5.51	123.05	120.30
1	L	356	TRP	CB-CG-CD1	-5.50	119.85	127.00
1	E	79	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	D	277	THR	CA-CB-CG2	5.42	119.98	112.40
1	J	210	ARG	CA-CB-CG	5.42	125.32	113.40
1	L	372	ARG	NE-CZ-NH2	-5.41	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	303	THR	CA-CB-CG2	5.38	119.94	112.40
1	F	79	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	D	340	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	J	69	TYR	CB-CG-CD2	-5.36	117.79	121.00
1	I	256	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	K	340	TRP	CG-CD2-CE3	5.34	138.71	133.90
1	E	169	TYR	CB-CG-CD2	-5.34	117.80	121.00
1	K	340	TRP	CB-CG-CD1	-5.34	120.06	127.00
1	N	306	TYR	CB-CG-CD2	-5.34	117.80	121.00
1	J	62	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	M	210	ARG	CA-CB-CG	5.32	125.10	113.40
1	A	340	TRP	CB-CG-CD1	-5.32	120.09	127.00
1	D	53	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	G	169	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	D	340	TRP	CB-CG-CD1	-5.30	120.10	127.00
1	F	282	ILE	CA-C-N	5.30	128.87	117.20
1	I	116	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	M	66	THR	CA-C-N	-5.30	105.54	117.20
1	L	340	TRP	CB-CG-CD1	-5.30	120.11	127.00
1	C	356	TRP	CB-CG-CD1	-5.29	120.12	127.00
1	L	147	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	K	62	ARG	CA-CB-CG	5.27	124.98	113.40
1	B	340	TRP	CB-CG-CD1	-5.26	120.16	127.00
1	L	290	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	J	72	GLU	CA-C-N	-5.26	105.63	117.20
1	K	356	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	G	222	ASP	N-CA-CB	5.25	120.06	110.60
1	D	202	THR	CA-CB-CG2	5.25	119.75	112.40
1	M	196	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	D	303	THR	CA-CB-CG2	5.25	119.74	112.40
1	F	306	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	L	79	TRP	CG-CD2-CE3	5.25	138.62	133.90
1	N	79	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	K	39	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	H	79	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	H	120	THR	CA-CB-OG1	-5.23	98.01	109.00
1	E	100	GLU	N-CA-CB	-5.22	101.19	110.60
1	M	79	TRP	CG-CD1-NE1	-5.22	104.88	110.10
1	G	79	TRP	CG-CD2-CE3	5.22	138.59	133.90
1	I	335	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	A	177	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	I	177	ARG	NE-CZ-NH1	-5.18	117.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	173	HIS	CA-CB-CG	5.17	122.39	113.60
1	N	37	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	79	TRP	CG-CD1-NE1	-5.17	104.93	110.10
1	G	254	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	I	39	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	340	TRP	CG-CD2-CE3	5.15	138.54	133.90
1	M	178	LEU	CA-CB-CG	5.15	127.15	115.30
1	N	39	ARG	NH1-CZ-NH2	-5.15	113.73	119.40
1	N	356	TRP	CG-CD2-CE3	5.15	138.53	133.90
1	M	86	TRP	CG-CD1-NE1	-5.14	104.96	110.10
1	J	37	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	79	TRP	CG-CD2-CE3	5.14	138.52	133.90
1	K	340	TRP	CG-CD1-NE1	-5.14	104.96	110.10
1	B	306	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	G	147	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	H	86	TRP	CG-CD1-NE1	-5.13	104.97	110.10
1	C	340	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	M	356	TRP	CB-CG-CD1	-5.11	120.36	127.00
1	I	356	TRP	CG-CD1-NE1	-5.10	105.00	110.10
1	H	340	TRP	CG-CD2-CE3	5.10	138.49	133.90
1	K	86	TRP	CG-CD1-NE1	-5.10	105.00	110.10
1	E	222	ASP	N-CA-CB	5.10	119.78	110.60
1	A	356	TRP	CG-CD1-NE1	-5.10	105.00	110.10
1	I	340	TRP	CG-CD2-CE3	5.09	138.48	133.90
1	M	312	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	N	197	GLY	CA-C-N	-5.08	106.03	117.20
1	I	62	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	N	275	HIS	CA-CB-CG	5.08	122.23	113.60
1	N	356	TRP	CG-CD1-NE1	-5.08	105.03	110.10
1	C	169	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	D	53	TYR	CA-CB-CG	5.07	123.04	113.40
1	A	62	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	C	198	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	E	356	TRP	CB-CG-CD1	-5.06	120.42	127.00
1	E	86	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	E	79	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	E	100	GLU	CA-CB-CG	5.05	124.50	113.40
1	E	237	GLU	N-CA-C	5.04	124.61	111.00
1	L	79	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	C	356	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	K	62	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	G	86	TRP	CG-CD1-NE1	-5.03	105.07	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	79	TRP	CG-CD1-NE1	-5.03	105.07	110.10
1	C	340	TRP	CG-CD2-CE3	5.02	138.42	133.90
1	J	340	TRP	CB-CG-CD1	-5.02	120.47	127.00
1	K	62	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	F	356	TRP	CB-CG-CD1	-5.02	120.48	127.00
1	F	183	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	I	340	TRP	CB-CG-CD1	-5.01	120.48	127.00
1	D	79	TRP	CG-CD2-CE3	5.00	138.40	133.90

There are no chirality outliers.

All (123) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	TYR	Sidechain
1	A	210	ARG	Sidechain
1	A	269	MET	Peptide
1	A	290	ARG	Sidechain
1	A	337	TYR	Sidechain
1	A	37	ARG	Sidechain
1	A	62	ARG	Sidechain
1	A	91	TYR	Sidechain
1	B	116	ARG	Sidechain
1	B	133	TYR	Sidechain
1	B	147	ARG	Sidechain
1	B	169	TYR	Sidechain
1	B	206	ARG	Sidechain
1	B	272	ALA	Peptide
1	B	28	ARG	Sidechain
1	B	285	CYS	Peptide
1	B	37	ARG	Sidechain
1	B	53	TYR	Sidechain
1	B	62	ARG	Sidechain
1	C	166	TYR	Sidechain
1	C	206	ARG	Sidechain
1	C	256	ARG	Sidechain
1	C	279	TYR	Sidechain
1	C	290	ARG	Sidechain
1	C	303	THR	Peptide
1	C	53	TYR	Sidechain
1	D	116	ARG	Sidechain
1	D	169	TYR	Sidechain
1	D	196	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	198	TYR	Sidechain
1	D	206	ARG	Sidechain
1	D	233	SER	Peptide
1	D	337	TYR	Sidechain
1	D	37	ARG	Sidechain
1	D	53	TYR	Sidechain
1	D	60	SER	Peptide
1	D	65	LEU	Peptide
1	E	111	ASN	Peptide
1	E	147	ARG	Sidechain
1	E	188	TYR	Sidechain
1	E	198	TYR	Sidechain
1	E	232	SER	Peptide
1	E	290	ARG	Sidechain
1	E	337	TYR	Sidechain
1	E	362	TYR	Sidechain
1	E	39	ARG	Sidechain
1	E	62	ARG	Sidechain
1	F	233	SER	Peptide
1	F	240	TYR	Sidechain
1	F	280	ASN	Peptide
1	F	281	SER	Peptide
1	F	282	ILE	Peptide
1	F	37	ARG	Sidechain
1	F	44	MET	Peptide
1	F	91	TYR	Sidechain
1	G	198	TYR	Sidechain
1	G	337	TYR	Sidechain
1	G	91	TYR	Sidechain
1	H	116	ARG	Sidechain
1	H	143	TYR	Sidechain
1	H	147	ARG	Sidechain
1	H	335	ARG	Sidechain
1	H	337	TYR	Sidechain
1	H	62	ARG	Sidechain
1	I	116	ARG	Sidechain
1	I	147	ARG	Sidechain
1	I	166	TYR	Sidechain
1	I	197	GLY	Peptide
1	I	252	ASN	Peptide
1	I	335	ARG	Sidechain
1	I	337	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	I	37	ARG	Sidechain
1	I	53	TYR	Sidechain
1	J	111	ASN	Peptide
1	J	196	ARG	Sidechain
1	J	202	THR	Peptide
1	J	205	GLU	Peptide
1	J	206	ARG	Sidechain
1	J	272	ALA	Peptide
1	J	290	ARG	Sidechain
1	J	306	TYR	Sidechain
1	K	116	ARG	Sidechain
1	K	147	ARG	Sidechain
1	K	166	TYR	Sidechain
1	K	206	ARG	Sidechain
1	K	218	TYR	Sidechain
1	K	240	TYR	Sidechain
1	K	290	ARG	Sidechain
1	K	303	THR	Peptide
1	K	337	TYR	Sidechain
1	K	37	ARG	Sidechain
1	K	53	TYR	Sidechain
1	K	91	TYR	Sidechain
1	L	116	ARG	Sidechain
1	L	169	TYR	Sidechain
1	L	179	ASP	Peptide
1	L	239	SER	Peptide
1	L	284	LYS	Peptide
1	L	289	ILE	Peptide
1	L	303	THR	Peptide
1	L	322	PRO	Peptide
1	L	337	TYR	Sidechain
1	L	39	ARG	Sidechain
1	L	53	TYR	Sidechain
1	L	62	ARG	Sidechain
1	L	65	LEU	Peptide
1	M	147	ARG	Sidechain
1	M	272	ALA	Peptide
1	M	337	TYR	Sidechain
1	M	39	ARG	Sidechain
1	M	53	TYR	Sidechain
1	M	62	ARG	Sidechain
1	M	91	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	N	143	TYR	Sidechain
1	N	147	ARG	Sidechain
1	N	196	ARG	Sidechain
1	N	254	ARG	Sidechain
1	N	275	HIS	Sidechain
1	N	306	TYR	Sidechain
1	N	37	ARG	Sidechain
1	N	53	TYR	Sidechain
1	N	62	ARG	Sidechain
1	N	91	TYR	Sidechain

## 4.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2933	0	2894	113	0
1	B	2933	0	2894	110	0
1	C	2933	0	2894	98	0
1	D	2933	0	2894	241	0
1	E	2933	0	2894	109	0
1	F	2933	0	2894	270	0
1	G	2933	0	2894	67	0
1	H	2933	0	2894	85	0
1	I	2933	0	2894	76	0
1	J	2933	0	2894	105	0
1	K	2933	0	2894	120	0
1	L	2933	0	2894	114	0
1	M	2933	0	2894	69	0
1	N	2933	0	2894	82	0
All	All	41062	0	40516	1305	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (1305) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:MET:CG	1:F:293:LEU:CD2	1.79	1.58
1:J:266:PHE:CE2	1:J:266:PHE:CZ	1.95	1.52
1:J:266:PHE:CD1	1:J:266:PHE:CE1	1.94	1.52
1:J:266:PHE:CG	1:J:266:PHE:CD1	1.95	1.52
1:J:266:PHE:CD2	1:J:266:PHE:CE2	1.95	1.51
1:J:266:PHE:CZ	1:J:266:PHE:CE1	1.95	1.51
1:D:44:MET:CG	1:F:293:LEU:HD21	1.06	1.50
1:J:266:PHE:CD2	1:J:266:PHE:CG	1.96	1.49
1:D:44:MET:SD	1:F:293:LEU:CD1	2.01	1.49
1:D:61:LYS:NZ	1:F:291:LYS:HD2	1.19	1.41
1:D:43:VAL:CB	1:F:166:TYR:HD1	1.34	1.39
1:L:112:PRO:N	1:L:112:PRO:CA	1.83	1.39
1:A:62:ARG:HH21	1:C:287:ILE:CD1	1.33	1.39
1:D:57:GLU:OE1	1:F:291:LYS:HE3	1.24	1.38
1:L:112:PRO:N	1:L:112:PRO:CD	1.88	1.35
1:A:62:ARG:NH2	1:C:287:ILE:HD11	1.37	1.34
1:D:65:LEU:N	1:F:287:ILE:HD11	1.39	1.33
1:D:64:ILE:C	1:F:287:ILE:HD11	1.45	1.32
1:D:61:LYS:NZ	1:F:291:LYS:CD	1.91	1.31
1:B:64:ILE:CG2	1:C:267:ILE:HB	1.59	1.31
1:D:44:MET:HG3	1:F:293:LEU:CD2	1.45	1.31
1:F:45:VAL:HG21	1:H:166:TYR:CE1	1.64	1.31
1:D:44:MET:SD	1:F:293:LEU:HD11	1.62	1.31
1:B:64:ILE:HG23	1:C:267:ILE:CB	1.63	1.26
1:L:112:PRO:CB	1:L:112:PRO:CG	2.12	1.25
1:L:112:PRO:CA	1:L:112:PRO:CB	2.13	1.25
1:A:62:ARG:HD2	1:C:287:ILE:CD1	1.68	1.23
1:D:43:VAL:HB	1:F:166:TYR:CD1	1.73	1.22
1:D:43:VAL:CB	1:F:166:TYR:CD1	2.25	1.18
1:D:65:LEU:N	1:F:287:ILE:CD1	2.06	1.18
1:L:112:PRO:CD	1:L:112:PRO:CG	2.22	1.18
1:F:45:VAL:CG2	1:H:166:TYR:CE1	2.24	1.18
1:D:44:MET:HG3	1:F:293:LEU:HD22	1.23	1.16
1:F:45:VAL:HA	1:H:167:GLU:CB	1.78	1.13
1:D:43:VAL:CG1	1:F:166:TYR:HD1	1.62	1.13
1:D:44:MET:SD	1:F:293:LEU:HD13	1.74	1.12
1:F:45:VAL:HA	1:H:167:GLU:HB2	1.23	1.12
1:D:57:GLU:OE1	1:F:291:LYS:CE	1.97	1.12
1:F:45:VAL:HG11	1:H:166:TYR:CE1	1.83	1.12
1:D:44:MET:HG2	1:F:293:LEU:CD2	1.56	1.11
1:D:65:LEU:HD23	1:F:287:ILE:HG13	1.22	1.10
1:B:50:LYS:HD3	1:B:53:TYR:OH	1.52	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:VAL:CG1	1:H:166:TYR:CE1	2.35	1.09
1:A:62:ARG:HD2	1:C:287:ILE:HD13	1.30	1.09
1:D:43:VAL:HG12	1:F:166:TYR:CD1	1.87	1.09
1:F:45:VAL:HG11	1:H:166:TYR:CZ	1.89	1.08
1:E:267:ILE:HD12	1:F:287:ILE:O	1.53	1.08
1:A:243:PRO:O	1:C:323:SER:N	1.86	1.08
1:D:43:VAL:HB	1:F:166:TYR:HD1	1.09	1.06
1:D:43:VAL:CG1	1:F:166:TYR:CD1	2.37	1.05
1:F:45:VAL:CG2	1:H:166:TYR:CD1	2.41	1.04
1:J:266:PHE:CZ	1:K:173:HIS:CG	2.46	1.02
1:J:266:PHE:CD1	1:K:173:HIS:CG	2.48	1.02
1:J:266:PHE:CE1	1:K:173:HIS:CG	2.47	1.02
1:J:266:PHE:CE2	1:K:173:HIS:CG	2.47	1.02
1:J:266:PHE:CG	1:K:173:HIS:CG	2.48	1.01
1:J:266:PHE:CD2	1:K:173:HIS:CG	2.48	1.00
1:D:45:VAL:HA	1:F:165:ILE:O	1.63	0.99
1:E:112:PRO:HB2	1:E:115:ASN:HB3	1.44	0.99
1:F:45:VAL:HG21	1:H:166:TYR:CD1	1.97	0.99
1:D:57:GLU:CD	1:F:291:LYS:HE3	1.85	0.97
1:F:45:VAL:CG1	1:H:166:TYR:CZ	2.50	0.95
1:D:64:ILE:HD11	1:F:286:ASP:HA	1.47	0.93
1:D:43:VAL:HG11	1:F:169:TYR:HD1	1.32	0.93
1:J:266:PHE:CD2	1:K:173:HIS:CB	2.52	0.92
1:D:64:ILE:HG13	1:F:287:ILE:HG12	1.49	0.92
1:D:45:VAL:HG13	1:F:165:ILE:HB	1.51	0.92
1:B:45:VAL:HG21	1:D:289:ILE:HD13	1.50	0.91
1:D:45:VAL:HG22	1:F:164:PRO:HA	1.52	0.91
1:F:45:VAL:HG11	1:H:166:TYR:OH	1.68	0.91
1:J:266:PHE:CG	1:K:173:HIS:CB	2.53	0.91
1:D:61:LYS:HZ2	1:F:291:LYS:CD	1.65	0.91
1:J:266:PHE:CE2	1:K:173:HIS:CB	2.54	0.91
1:J:266:PHE:CE1	1:K:173:HIS:CB	2.54	0.91
1:F:45:VAL:HG22	1:H:166:TYR:CD1	2.05	0.90
1:J:266:PHE:CZ	1:K:173:HIS:CB	2.55	0.90
1:D:61:LYS:HZ1	1:F:291:LYS:CD	1.76	0.89
1:F:45:VAL:HG21	1:H:166:TYR:HE1	1.12	0.89
1:J:266:PHE:CD2	1:K:173:HIS:HB2	2.06	0.89
1:J:266:PHE:CD1	1:K:173:HIS:CB	2.54	0.89
1:D:64:ILE:CA	1:F:287:ILE:HD11	2.02	0.89
1:K:192:ILE:HA	1:L:112:PRO:HG3	1.54	0.88
1:B:45:VAL:HG13	1:D:171:LEU:HB2	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ARG:HD3	1:B:66:THR:HG23	1.55	0.87
1:D:45:VAL:HG11	1:F:142:LEU:HD13	1.56	0.87
1:D:64:ILE:CD1	1:F:286:ASP:HA	2.05	0.87
1:D:65:LEU:H	1:F:287:ILE:CD1	1.84	0.87
1:A:357:ILE:HG13	1:A:370:VAL:HG22	1.55	0.86
1:D:44:MET:CE	1:F:293:LEU:HD13	2.06	0.86
1:D:43:VAL:HA	1:F:166:TYR:CE1	2.10	0.86
1:D:44:MET:O	1:F:165:ILE:N	2.09	0.85
1:K:195:GLU:CB	1:L:112:PRO:N	2.39	0.85
1:E:267:ILE:HG23	1:F:290:ARG:HB2	1.59	0.85
1:B:63:GLY:HA3	1:C:267:ILE:HA	1.58	0.84
1:N:102:PRO:HB3	1:N:131:ALA:HB3	1.58	0.84
1:F:154:ASP:HB3	1:F:161:HIS:HB2	1.59	0.84
1:J:266:PHE:CD1	1:K:173:HIS:HB3	2.12	0.84
1:B:102:PRO:HB3	1:B:131:ALA:HB3	1.59	0.84
1:L:160:THR:HB	1:L:178:LEU:HB3	1.59	0.83
1:A:62:ARG:CD	1:C:287:ILE:CD1	2.54	0.83
1:A:62:ARG:HG3	1:C:286:ASP:HB2	1.58	0.83
1:D:44:MET:HB2	1:F:289:ILE:CG2	2.10	0.82
1:A:243:PRO:HB2	1:C:322:PRO:HB2	1.62	0.82
1:K:195:GLU:CG	1:L:112:PRO:N	2.43	0.82
1:A:102:PRO:HB3	1:A:131:ALA:HB3	1.62	0.81
1:A:257:CYS:SG	1:A:258:PRO:HD3	2.20	0.81
1:J:19:ALA:HB3	1:J:29:ALA:HB3	1.61	0.81
1:D:61:LYS:HZ3	1:F:291:LYS:HD2	1.40	0.81
1:K:195:GLU:CG	1:L:112:PRO:CA	2.59	0.81
1:C:160:THR:HB	1:C:178:LEU:HB2	1.62	0.81
1:K:195:GLU:CB	1:L:112:PRO:CD	2.59	0.81
1:B:63:GLY:H	1:C:268:GLY:H	1.25	0.81
1:A:62:ARG:HD2	1:C:287:ILE:HD11	1.64	0.80
1:D:47:MET:O	1:F:166:TYR:HD2	1.65	0.79
1:E:267:ILE:CD1	1:F:287:ILE:O	2.30	0.79
1:K:195:GLU:CG	1:L:112:PRO:CD	2.61	0.79
1:E:267:ILE:CG2	1:F:290:ARG:HB2	2.14	0.78
1:G:257:CYS:SG	1:G:258:PRO:HD3	2.24	0.78
1:H:164:PRO:HG3	1:H:174:ALA:HB3	1.64	0.78
1:L:19:ALA:HB3	1:L:29:ALA:HB3	1.65	0.78
1:D:64:ILE:N	1:F:287:ILE:HD13	1.99	0.77
1:N:36:GLY:HA2	1:N:66:THR:HB	1.64	0.77
1:D:65:LEU:H	1:F:287:ILE:HD12	1.49	0.77
1:D:64:ILE:N	1:F:287:ILE:CD1	2.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:MET:SD	1:F:293:LEU:CD2	2.71	0.77
1:K:195:GLU:CB	1:L:112:PRO:CA	2.62	0.77
1:D:47:MET:O	1:F:166:TYR:CD2	2.38	0.77
1:D:43:VAL:CA	1:F:166:TYR:CD1	2.69	0.76
1:F:45:VAL:HG13	1:H:167:GLU:HG2	1.68	0.76
1:M:160:THR:HB	1:M:178:LEU:HB2	1.68	0.76
1:E:206:ARG:HG3	1:F:264:PRO:HB2	1.68	0.75
1:D:44:MET:CG	1:F:293:LEU:HD22	1.90	0.75
1:B:63:GLY:N	1:C:268:GLY:H	1.84	0.75
1:A:38:PRO:HA	1:A:65:LEU:HA	1.67	0.75
1:B:45:VAL:HG22	1:D:171:LEU:HD12	1.68	0.75
1:A:62:ARG:NH2	1:C:287:ILE:CD1	2.18	0.75
1:A:62:ARG:HH21	1:C:287:ILE:HD11	0.61	0.75
1:B:257:CYS:SG	1:B:258:PRO:HD3	2.26	0.75
1:C:200:PHE:HB3	1:C:206:ARG:HG2	1.69	0.74
1:K:195:GLU:CG	1:L:112:PRO:CG	2.64	0.74
1:D:65:LEU:N	1:F:287:ILE:HD12	2.03	0.74
1:F:163:VAL:HG13	1:F:175:ILE:HG12	1.68	0.74
1:B:63:GLY:CA	1:C:267:ILE:HA	2.17	0.74
1:D:257:CYS:SG	1:D:258:PRO:HD3	2.28	0.74
1:H:257:CYS:SG	1:H:258:PRO:HD3	2.27	0.74
1:N:19:ALA:HB3	1:N:29:ALA:HB3	1.69	0.74
1:C:19:ALA:HB3	1:C:29:ALA:HB3	1.70	0.73
1:B:164:PRO:HG2	1:B:171:LEU:HB3	1.69	0.73
1:F:45:VAL:CA	1:H:167:GLU:HB2	2.12	0.73
1:G:267:ILE:CD1	1:H:169:TYR:OH	2.37	0.73
1:D:43:VAL:HA	1:F:166:TYR:CD1	2.23	0.73
1:K:195:GLU:CG	1:L:112:PRO:CB	2.67	0.73
1:K:195:GLU:CB	1:L:112:PRO:CG	2.66	0.73
1:K:195:GLU:CB	1:L:112:PRO:CB	2.67	0.73
1:A:62:ARG:CZ	1:C:287:ILE:HD11	2.17	0.73
1:F:195:GLU:HA	1:G:172:PRO:HB2	1.71	0.72
1:D:43:VAL:CA	1:F:166:TYR:HD1	2.02	0.72
1:F:36:GLY:HA3	1:F:65:LEU:HD13	1.71	0.72
1:B:160:THR:HB	1:B:178:LEU:HB3	1.71	0.72
1:H:357:ILE:HG13	1:H:370:VAL:HG22	1.71	0.72
1:D:64:ILE:HG13	1:F:287:ILE:CG1	2.20	0.72
1:L:357:ILE:HG13	1:L:370:VAL:HG22	1.72	0.72
1:C:257:CYS:SG	1:C:258:PRO:HD3	2.29	0.71
1:D:61:LYS:HZ1	1:F:291:LYS:HB3	1.54	0.71
1:D:191:LYS:HE2	1:E:172:PRO:HG2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:VAL:HB	1:F:150:GLY:H	1.55	0.71
1:B:163:VAL:HG22	1:B:175:ILE:HG23	1.72	0.71
1:B:60:SER:O	1:D:287:ILE:HG21	1.91	0.71
1:D:47:MET:O	1:F:167:GLU:HG2	1.91	0.71
1:M:102:PRO:HB3	1:M:131:ALA:HB3	1.70	0.71
1:N:24:ASP:HB2	1:N:340:TRP:HH2	1.54	0.71
1:B:38:PRO:HA	1:B:65:LEU:HA	1.73	0.71
1:L:244:ASP:HB2	1:L:245:GLY:HA2	1.73	0.71
1:F:45:VAL:HG13	1:H:167:GLU:CG	2.20	0.71
1:I:257:CYS:SG	1:I:258:PRO:HD3	2.30	0.71
1:E:199:SER:HB2	1:F:179:ASP:HB2	1.72	0.70
1:J:266:PHE:CG	1:K:173:HIS:HB3	2.26	0.70
1:D:61:LYS:HZ2	1:F:291:LYS:HD2	0.77	0.70
1:E:183:ARG:HG3	1:F:270:GLU:HG2	1.73	0.70
1:D:65:LEU:CD2	1:F:287:ILE:HG21	2.21	0.70
1:A:174:ALA:HA	1:A:284:LYS:HE2	1.73	0.70
1:F:19:ALA:HB3	1:F:29:ALA:HB3	1.74	0.70
1:K:191:LYS:HE2	1:L:110:LEU:HD22	1.72	0.70
1:B:39:ARG:HD3	1:B:66:THR:CG2	2.22	0.70
1:D:61:LYS:NZ	1:F:291:LYS:HD3	2.00	0.69
1:D:64:ILE:C	1:F:287:ILE:CD1	2.42	0.69
1:L:204:ALA:HA	1:N:287:ILE:HD12	1.75	0.69
1:E:257:CYS:SG	1:E:258:PRO:HD3	2.32	0.69
1:N:164:PRO:HG3	1:N:174:ALA:HB3	1.73	0.69
1:L:190:MET:HA	1:L:209:VAL:HG11	1.74	0.69
1:D:44:MET:HE1	1:F:293:LEU:HD13	1.75	0.69
1:D:61:LYS:NZ	1:F:291:LYS:HB3	2.06	0.69
1:N:265:SER:HA	1:N:270:GLU:HA	1.74	0.69
1:A:62:ARG:HG3	1:C:286:ASP:CB	2.22	0.69
1:D:282:ILE:HA	1:D:285:CYS:SG	2.33	0.69
1:K:194:THR:HB	1:L:75:ILE:HG12	1.75	0.69
1:N:160:THR:HB	1:N:178:LEU:HB2	1.75	0.69
1:D:197:GLY:HA2	1:E:112:PRO:HA	1.72	0.68
1:H:285:CYS:HB3	1:H:289:ILE:HD11	1.76	0.68
1:J:180:LEU:HD11	1:J:264:PRO:HB3	1.73	0.68
1:K:264:PRO:HB2	1:K:271:SER:HB3	1.76	0.68
1:D:58:ALA:O	1:D:62:ARG:HB3	1.93	0.68
1:J:266:PHE:CD2	1:K:173:HIS:CD2	2.82	0.68
1:F:213:LYS:HA	1:F:217:CYS:SG	2.34	0.68
1:D:45:VAL:HG13	1:F:165:ILE:CB	2.25	0.67
1:D:53:TYR:HB2	1:F:288:ASP:OD1	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:VAL:HG22	1:F:175:ILE:HG23	1.76	0.67
1:D:64:ILE:CA	1:F:287:ILE:CD1	2.70	0.67
1:D:65:LEU:HD23	1:F:287:ILE:CG1	2.14	0.67
1:F:45:VAL:HG11	1:H:166:TYR:HE1	1.54	0.67
1:J:160:THR:HB	1:J:178:LEU:HB2	1.76	0.67
1:D:49:GLN:N	1:F:166:TYR:CD2	2.62	0.67
1:D:44:MET:HB2	1:F:289:ILE:HG21	1.76	0.67
1:I:191:LYS:HE2	1:J:172:PRO:HB2	1.77	0.67
1:L:242:LEU:HB2	1:L:245:GLY:HA3	1.76	0.67
1:L:300:SER:HA	1:L:335:ARG:HB2	1.77	0.67
1:D:57:GLU:CD	1:F:291:LYS:CE	2.54	0.66
1:I:19:ALA:HB3	1:I:29:ALA:HB3	1.76	0.66
1:J:193:LEU:HA	1:J:196:ARG:HB3	1.77	0.66
1:L:257:CYS:SG	1:L:258:PRO:HD3	2.35	0.66
1:L:36:GLY:HA3	1:L:65:LEU:HD13	1.77	0.66
1:M:9:VAL:HG21	1:M:344:SER:HA	1.78	0.66
1:D:43:VAL:HA	1:F:166:TYR:HE1	1.57	0.66
1:E:210:ARG:HB2	1:F:269:MET:SD	2.36	0.66
1:G:286:ASP:HB3	1:G:289:ILE:HG12	1.77	0.66
1:N:266:PHE:HB3	1:N:269:MET:SD	2.35	0.66
1:D:45:VAL:HG13	1:F:165:ILE:CD1	2.24	0.66
1:I:180:LEU:HD11	1:I:264:PRO:HB3	1.76	0.66
1:D:201:VAL:HB	1:E:177:ARG:HB3	1.76	0.66
1:B:64:ILE:HD13	1:C:267:ILE:HD12	1.76	0.66
1:F:45:VAL:HG13	1:H:166:TYR:CZ	2.31	0.66
1:N:106:THR:HG22	1:N:140:LEU:HD12	1.78	0.66
1:F:160:THR:HB	1:F:178:LEU:HB3	1.77	0.65
1:I:189:LEU:HA	1:I:192:ILE:HG12	1.78	0.65
1:D:102:PRO:HB3	1:D:131:ALA:HB3	1.78	0.65
1:E:10:CYS:SG	1:E:89:THR:HG21	2.37	0.65
1:F:45:VAL:CG1	1:H:166:TYR:OH	2.39	0.65
1:A:285:CYS:HB3	1:A:289:ILE:HD11	1.79	0.65
1:E:116:ARG:NH2	1:E:374:CYS:SG	2.70	0.65
1:F:257:CYS:SG	1:F:258:PRO:HD3	2.37	0.65
1:G:7:ALA:HA	1:G:102:PRO:HG2	1.79	0.65
1:I:102:PRO:HB3	1:I:131:ALA:HB3	1.79	0.65
1:K:357:ILE:HG13	1:K:370:VAL:HG22	1.78	0.65
1:A:243:PRO:HB2	1:C:322:PRO:CB	2.27	0.65
1:F:46:GLY:H	1:H:167:GLU:HB3	1.62	0.64
1:F:45:VAL:CB	1:H:166:TYR:CE1	2.80	0.64
1:D:213:LYS:HA	1:D:217:CYS:SG	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:VAL:HG11	1:F:166:TYR:HB2	1.78	0.64
1:D:44:MET:HB2	1:F:289:ILE:HG22	1.79	0.64
1:K:244:ASP:HB3	1:M:287:ILE:O	1.98	0.64
1:L:111:ASN:C	1:L:112:PRO:CA	2.64	0.64
1:B:213:LYS:HA	1:B:217:CYS:SG	2.38	0.64
1:D:65:LEU:HD21	1:F:287:ILE:HG21	1.79	0.64
1:N:257:CYS:SG	1:N:258:PRO:HD3	2.38	0.64
1:B:45:VAL:HB	1:D:166:TYR:HB3	1.79	0.64
1:D:57:GLU:OE2	1:F:291:LYS:CE	2.46	0.64
1:F:45:VAL:CA	1:H:167:GLU:CB	2.68	0.64
1:I:164:PRO:HG3	1:I:174:ALA:HB3	1.79	0.64
1:N:155:SER:HA	1:N:160:THR:HA	1.80	0.64
1:G:213:LYS:HA	1:G:217:CYS:SG	2.38	0.63
1:M:10:CYS:SG	1:M:89:THR:HG21	2.37	0.63
1:A:137:GLN:HG2	1:A:339:VAL:HG11	1.80	0.63
1:C:267:ILE:HG21	1:D:284:LYS:HG3	1.80	0.63
1:C:245:GLY:H	1:E:325:MET:HB2	1.63	0.63
1:J:266:PHE:CE1	1:K:173:HIS:ND1	2.66	0.63
1:K:160:THR:HB	1:K:178:LEU:HB2	1.80	0.63
1:E:357:ILE:HG21	1:E:370:VAL:HG22	1.79	0.63
1:M:257:CYS:SG	1:M:258:PRO:HD3	2.38	0.63
1:N:162:ASN:OD1	1:N:277:THR:HG23	1.99	0.63
1:B:109:PRO:HA	1:B:136:ILE:HG23	1.80	0.63
1:D:43:VAL:HG11	1:F:169:TYR:CD1	2.23	0.63
1:D:44:MET:HG2	1:F:293:LEU:HD21	0.64	0.63
1:F:45:VAL:C	1:H:167:GLU:HG3	2.19	0.63
1:K:164:PRO:HG2	1:K:171:LEU:HB2	1.81	0.63
1:L:289:ILE:HA	1:L:291:LYS:HG2	1.81	0.62
1:N:66:THR:HG22	1:N:68:LYS:HG2	1.80	0.62
1:E:160:THR:HB	1:E:178:LEU:HB2	1.81	0.62
1:N:357:ILE:HG13	1:N:370:VAL:HG22	1.81	0.62
1:G:9:VAL:HG21	1:G:344:SER:HA	1.80	0.62
1:N:200:PHE:HA	1:N:205:GLU:HB3	1.82	0.62
1:B:60:SER:OG	1:D:287:ILE:HD13	1.99	0.62
1:D:197:GLY:HA2	1:E:113:LYS:H	1.64	0.62
1:E:62:ARG:HB2	1:E:62:ARG:HH21	1.65	0.62
1:D:45:VAL:CG1	1:F:165:ILE:CD1	2.78	0.62
1:D:160:THR:HB	1:D:178:LEU:HB3	1.82	0.62
1:I:242:LEU:HD11	1:I:248:ILE:HD13	1.80	0.62
1:K:205:GLU:HG2	1:M:287:ILE:HG13	1.82	0.62
1:D:36:GLY:HA3	1:D:65:LEU:HD22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:160:THR:HB	1:H:178:LEU:HB2	1.81	0.62
1:D:298:VAL:HG22	1:D:330:ILE:HB	1.82	0.62
1:B:63:GLY:HA3	1:C:268:GLY:N	2.15	0.62
1:A:10:CYS:HB3	1:A:105:LEU:HD23	1.80	0.61
1:A:153:LEU:HD21	1:A:274:ILE:HG23	1.81	0.61
1:C:178:LEU:HD11	1:C:277:THR:HG21	1.81	0.61
1:N:103:THR:O	1:N:132:MET:HA	2.00	0.61
1:C:328:LYS:HZ1	1:C:330:ILE:HG12	1.63	0.61
1:D:47:MET:C	1:F:167:GLU:HG2	2.21	0.61
1:A:36:GLY:HA2	1:A:66:THR:O	2.00	0.61
1:D:61:LYS:HZ1	1:F:291:LYS:HD3	1.58	0.61
1:E:287:ILE:HD12	1:E:287:ILE:H	1.65	0.61
1:J:153:LEU:HA	1:J:161:HIS:O	2.00	0.61
1:N:189:LEU:HD13	1:N:257:CYS:SG	2.40	0.61
1:F:45:VAL:HA	1:H:167:GLU:HB3	1.78	0.61
1:D:44:MET:HE2	1:F:293:LEU:HD22	1.82	0.61
1:F:46:GLY:N	1:H:167:GLU:HG3	2.15	0.61
1:F:45:VAL:CG2	1:H:166:TYR:HE1	1.83	0.61
1:J:105:LEU:HB2	1:J:134:VAL:HG12	1.82	0.61
1:I:63:GLY:HA3	1:J:268:GLY:H	1.66	0.61
1:F:248:ILE:HG23	1:F:250:ILE:HD11	1.81	0.61
1:D:65:LEU:CD2	1:F:287:ILE:HG13	2.14	0.61
1:D:43:VAL:CG1	1:F:169:TYR:HD1	2.08	0.61
1:J:266:PHE:CZ	1:K:173:HIS:ND1	2.68	0.61
1:E:265:SER:HB3	1:F:285:CYS:HA	1.81	0.61
1:F:45:VAL:HG13	1:H:166:TYR:CE1	2.33	0.60
1:L:189:LEU:HA	1:L:192:ILE:HG12	1.83	0.60
1:D:170:ALA:HB1	1:D:175:ILE:HD11	1.83	0.60
1:J:205:GLU:HA	1:L:288:ASP:HB2	1.82	0.60
1:M:34:ILE:HG21	1:M:67:LEU:HB3	1.83	0.60
1:C:203:THR:HG21	1:D:267:ILE:HG23	1.84	0.60
1:D:57:GLU:OE2	1:F:291:LYS:HD2	2.02	0.60
1:K:63:GLY:HA3	1:L:267:ILE:HA	1.83	0.60
1:C:9:VAL:HG21	1:C:344:SER:HA	1.83	0.60
1:J:266:PHE:HE1	1:K:171:LEU:HB3	1.66	0.60
1:L:305:MET:SD	1:L:336:LYS:HB3	2.42	0.60
1:E:189:LEU:HD13	1:E:257:CYS:SG	2.42	0.60
1:K:164:PRO:HG3	1:K:174:ALA:HB3	1.84	0.60
1:A:189:LEU:HD13	1:A:257:CYS:SG	2.42	0.60
1:A:32:PRO:HB2	1:A:34:ILE:HG12	1.84	0.60
1:D:120:THR:HG21	1:D:370:VAL:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:205:GLU:HB3	1:L:289:ILE:H	1.66	0.60
1:L:164:PRO:HG2	1:L:171:LEU:HB2	1.83	0.60
1:C:11:ASP:HB3	1:C:18:LYS:HB2	1.84	0.60
1:B:63:GLY:CA	1:C:268:GLY:H	2.14	0.60
1:G:170:ALA:O	1:G:172:PRO:HD3	2.01	0.60
1:I:9:VAL:HG21	1:I:344:SER:HA	1.84	0.60
1:K:32:PRO:HB2	1:K:34:ILE:HG12	1.83	0.60
1:M:282:ILE:HG12	1:M:293:LEU:HD23	1.83	0.60
1:A:160:THR:HB	1:A:178:LEU:HB3	1.84	0.60
1:K:10:CYS:HA	1:K:18:LYS:O	2.02	0.60
1:J:266:PHE:CE2	1:K:173:HIS:HB2	2.37	0.59
1:C:357:ILE:HG21	1:C:370:VAL:HG22	1.84	0.59
1:E:213:LYS:HA	1:E:217:CYS:SG	2.42	0.59
1:J:266:PHE:CG	1:K:173:HIS:CD2	2.90	0.59
1:L:155:SER:HA	1:L:160:THR:HA	1.84	0.59
1:H:190:MET:SD	1:H:209:VAL:HG21	2.42	0.59
1:J:266:PHE:CE1	1:K:171:LEU:HB3	2.37	0.59
1:D:44:MET:SD	1:F:293:LEU:CG	2.87	0.59
1:C:86:TRP:HH2	1:C:119:MET:HG2	1.68	0.59
1:B:63:GLY:HA3	1:C:267:ILE:CA	2.31	0.59
1:C:328:LYS:NZ	1:C:330:ILE:HG12	2.18	0.59
1:E:207:GLU:HB3	1:F:269:MET:H	1.68	0.59
1:L:219:VAL:HG22	1:L:258:PRO:HB3	1.84	0.59
1:A:103:THR:O	1:A:132:MET:HA	2.03	0.59
1:A:203:THR:OG1	1:C:287:ILE:HG23	2.03	0.58
1:E:250:ILE:HG23	1:E:253:GLU:HB2	1.85	0.58
1:F:70:PRO:HG3	1:F:85:ILE:HD12	1.85	0.58
1:J:203:THR:HB	1:K:268:GLY:HA3	1.85	0.58
1:K:195:GLU:HG2	1:L:112:PRO:CG	2.33	0.58
1:D:47:MET:HA	1:F:167:GLU:OE2	2.03	0.58
1:G:102:PRO:HB3	1:G:131:ALA:HB3	1.84	0.58
1:K:153:LEU:HD21	1:K:274:ILE:HG23	1.85	0.58
1:A:53:TYR:CZ	1:A:61:LYS:CD	2.86	0.58
1:E:164:PRO:HG2	1:E:171:LEU:HB2	1.85	0.58
1:G:189:LEU:HD12	1:G:192:ILE:HD11	1.85	0.58
1:D:64:ILE:HG13	1:F:287:ILE:CD1	2.34	0.58
1:A:19:ALA:HB3	1:A:29:ALA:HB3	1.84	0.58
1:J:7:ALA:HA	1:J:102:PRO:HG2	1.86	0.58
1:E:10:CYS:HB3	1:E:105:LEU:HD23	1.85	0.58
1:I:153:LEU:HA	1:I:161:HIS:O	2.03	0.58
1:J:120:THR:HG21	1:J:370:VAL:HG21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:219:VAL:HG21	1:J:309:ILE:HB	1.86	0.58
1:D:38:PRO:HB3	1:D:64:ILE:HD12	1.86	0.58
1:A:53:TYR:CZ	1:A:61:LYS:HD2	2.39	0.58
1:I:240:TYR:HB3	1:I:248:ILE:HG22	1.85	0.58
1:C:205:GLU:N	1:E:287:ILE:HD13	2.19	0.57
1:D:44:MET:O	1:F:165:ILE:C	2.42	0.57
1:D:48:GLY:C	1:F:166:TYR:CE2	2.78	0.57
1:I:286:ASP:O	1:I:290:ARG:HG3	2.04	0.57
1:C:207:GLU:O	1:C:210:ARG:HB2	2.04	0.57
1:G:109:PRO:HA	1:G:136:ILE:HG23	1.85	0.57
1:A:153:LEU:HA	1:A:161:HIS:O	2.05	0.57
1:J:213:LYS:HA	1:J:217:CYS:SG	2.45	0.57
1:L:213:LYS:HA	1:L:217:CYS:SG	2.43	0.57
1:B:194:THR:HG22	1:B:198:TYR:O	2.04	0.57
1:D:61:LYS:HZ1	1:F:291:LYS:CB	2.16	0.57
1:D:33:SER:O	1:D:70:PRO:HD2	2.04	0.57
1:I:164:PRO:HG2	1:I:171:LEU:HB2	1.85	0.57
1:I:98:PRO:HB2	1:I:129:VAL:HG12	1.87	0.57
1:E:19:ALA:HB3	1:E:29:ALA:HB3	1.85	0.57
1:G:160:THR:HB	1:G:178:LEU:HB3	1.86	0.57
1:M:151:ILE:HB	1:M:293:LEU:HG	1.86	0.57
1:A:165:ILE:HG12	1:A:170:ALA:HA	1.87	0.57
1:D:194:THR:HG22	1:D:198:TYR:H	1.70	0.57
1:F:9:VAL:HG21	1:F:344:SER:HA	1.85	0.57
1:K:195:GLU:HB3	1:L:112:PRO:N	2.19	0.57
1:K:62:ARG:HG3	1:K:67:LEU:HD11	1.87	0.57
1:B:165:ILE:HA	1:B:170:ALA:HA	1.86	0.57
1:C:163:VAL:HG22	1:C:175:ILE:HG23	1.87	0.57
1:E:268:GLY:H	1:F:290:ARG:HE	1.51	0.57
1:K:195:GLU:HG3	1:L:112:PRO:CA	2.35	0.57
1:B:63:GLY:HA3	1:C:268:GLY:H	1.70	0.56
1:G:10:CYS:HA	1:G:18:LYS:O	2.04	0.56
1:A:9:VAL:HG21	1:A:344:SER:HA	1.86	0.56
1:D:359:LYS:HD2	1:D:360:GLN:HB2	1.87	0.56
1:L:330:ILE:O	1:L:332:PRO:HD3	2.05	0.56
1:N:213:LYS:HA	1:N:217:CYS:SG	2.45	0.56
1:A:37:ARG:O	1:A:66:THR:N	2.37	0.56
1:J:9:VAL:HG21	1:J:344:SER:HA	1.87	0.56
1:D:44:MET:CG	1:F:293:LEU:CG	2.77	0.56
1:K:153:LEU:HA	1:K:161:HIS:O	2.05	0.56
1:E:153:LEU:HA	1:E:161:HIS:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:142:LEU:HG	1:G:147:ARG:HB2	1.87	0.56
1:B:286:ASP:HB3	1:B:289:ILE:HD11	1.88	0.56
1:K:188:TYR:HE2	1:K:257:CYS:HA	1.71	0.56
1:L:75:ILE:HD11	1:L:177:ARG:HH22	1.70	0.56
1:N:135:ALA:HB3	1:N:140:LEU:HD11	1.88	0.56
1:A:98:PRO:HB2	1:A:127:PHE:O	2.06	0.56
1:A:152:VAL:O	1:A:162:ASN:HA	2.06	0.55
1:A:262:PHE:O	1:A:275:HIS:HE1	1.88	0.55
1:B:104:LEU:HG	1:B:133:TYR:HB3	1.89	0.55
1:J:359:LYS:HD2	1:J:360:GLN:HB2	1.87	0.55
1:K:286:ASP:O	1:K:290:ARG:HG3	2.07	0.55
1:A:252:ASN:H	1:A:252:ASN:ND2	2.04	0.55
1:E:190:MET:SD	1:F:272:ALA:HB3	2.47	0.55
1:G:148:THR:HB	1:G:167:GLU:HA	1.88	0.55
1:I:103:THR:O	1:I:132:MET:HA	2.06	0.55
1:K:213:LYS:HD3	1:K:214:GLU:HG3	1.89	0.55
1:L:369:ILE:HA	1:L:372:ARG:HB2	1.89	0.55
1:E:198:TYR:CZ	1:E:248:ILE:HA	2.41	0.55
1:G:242:LEU:HG	1:G:243:PRO:HD2	1.87	0.55
1:I:10:CYS:HB3	1:I:105:LEU:HD23	1.89	0.55
1:J:164:PRO:HG2	1:J:171:LEU:HB2	1.87	0.55
1:B:63:GLY:HA3	1:C:266:PHE:O	2.07	0.55
1:J:303:THR:HG23	1:J:306:TYR:HE2	1.72	0.55
1:G:44:MET:HB2	1:G:47:MET:HB2	1.89	0.55
1:H:359:LYS:HD2	1:H:360:GLN:HB2	1.86	0.55
1:L:280:ASN:HA	1:L:283:MET:HB3	1.87	0.55
1:B:300:SER:HA	1:B:335:ARG:HB2	1.88	0.55
1:C:244:ASP:HB3	1:E:287:ILE:HG23	1.88	0.55
1:F:7:ALA:HA	1:F:102:PRO:HG2	1.89	0.55
1:B:238:LYS:HA	1:B:238:LYS:HE3	1.88	0.55
1:H:162:ASN:OD1	1:H:277:THR:HG23	2.07	0.55
1:I:32:PRO:HB2	1:I:34:ILE:HG12	1.89	0.55
1:D:7:ALA:HA	1:D:102:PRO:HG2	1.89	0.55
1:D:46:GLY:HA2	1:F:149:THR:HG23	1.89	0.55
1:C:7:ALA:HA	1:C:102:PRO:HG2	1.88	0.54
1:D:45:VAL:HG11	1:F:142:LEU:CD1	2.34	0.54
1:F:188:TYR:HA	1:F:191:LYS:HD3	1.88	0.54
1:L:32:PRO:HB2	1:L:34:ILE:HG12	1.88	0.54
1:D:44:MET:CE	1:F:293:LEU:HD22	2.38	0.54
1:K:106:THR:HG22	1:K:140:LEU:HD12	1.89	0.54
1:L:64:ILE:HG13	1:L:65:LEU:HG	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:THR:HB	1:A:167:GLU:HA	1.90	0.54
1:D:357:ILE:HG21	1:D:370:VAL:HG22	1.88	0.54
1:E:153:LEU:HD21	1:E:274:ILE:HD12	1.89	0.54
1:I:190:MET:SD	1:I:209:VAL:HG21	2.48	0.54
1:J:98:PRO:HB2	1:J:129:VAL:HG12	1.88	0.54
1:M:103:THR:O	1:M:132:MET:HA	2.07	0.54
1:N:330:ILE:O	1:N:332:PRO:HD3	2.08	0.54
1:F:140:LEU:HD22	1:F:343:GLY:HA2	1.89	0.54
1:D:43:VAL:HG21	1:F:169:TYR:O	2.07	0.54
1:G:10:CYS:HB3	1:G:105:LEU:HD23	1.90	0.54
1:C:189:LEU:HD13	1:C:257:CYS:SG	2.48	0.54
1:E:190:MET:HA	1:E:209:VAL:HG11	1.90	0.54
1:D:61:LYS:HA	1:E:268:GLY:HA2	1.89	0.54
1:F:161:HIS:HA	1:F:176:MET:O	2.08	0.54
1:J:162:ASN:O	1:J:175:ILE:HA	2.07	0.54
1:K:162:ASN:OD1	1:K:277:THR:HG23	2.06	0.54
1:B:103:THR:O	1:B:132:MET:HA	2.07	0.54
1:D:62:ARG:O	1:E:270:GLU:HA	2.08	0.54
1:A:203:THR:OG1	1:C:287:ILE:CG2	2.56	0.54
1:A:304:THR:O	1:A:309:ILE:HG21	2.07	0.54
1:F:304:THR:O	1:F:309:ILE:HG21	2.07	0.54
1:K:330:ILE:O	1:K:332:PRO:HD3	2.08	0.54
1:N:98:PRO:HB2	1:N:127:PHE:O	2.08	0.54
1:N:190:MET:O	1:N:194:THR:HG23	2.08	0.54
1:D:203:THR:HG21	1:E:269:MET:HA	1.90	0.54
1:D:44:MET:HG2	1:F:293:LEU:CG	2.32	0.54
1:E:304:THR:HA	1:E:309:ILE:HD13	1.90	0.54
1:H:162:ASN:O	1:H:175:ILE:HA	2.08	0.54
1:B:162:ASN:O	1:B:175:ILE:HA	2.08	0.54
1:D:57:GLU:OE2	1:F:291:LYS:HE3	2.04	0.54
1:M:109:PRO:HA	1:M:136:ILE:HG23	1.90	0.54
1:A:114:ALA:HA	1:A:117:GLU:HB2	1.88	0.53
1:C:305:MET:SD	1:C:336:LYS:HD3	2.49	0.53
1:G:359:LYS:HD2	1:G:360:GLN:HB2	1.89	0.53
1:A:299:MET:SD	1:A:313:MET:HG3	2.48	0.53
1:C:102:PRO:HB3	1:C:131:ALA:HB3	1.90	0.53
1:B:330:ILE:O	1:B:332:PRO:HD3	2.08	0.53
1:H:163:VAL:HG22	1:H:175:ILE:HG23	1.91	0.53
1:K:197:GLY:O	1:L:77:THR:HA	2.08	0.53
1:D:239:SER:HA	1:D:248:ILE:O	2.07	0.53
1:E:180:LEU:HD21	1:F:283:MET:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:359:LYS:HD2	1:F:360:GLN:HB2	1.90	0.53
1:N:300:SER:HA	1:N:335:ARG:HB2	1.90	0.53
1:A:186:THR:HG21	1:A:210:ARG:HB3	1.91	0.53
1:D:43:VAL:HG22	1:F:171:LEU:HG	1.89	0.53
1:D:45:VAL:CA	1:F:165:ILE:O	2.49	0.53
1:K:19:ALA:HB3	1:K:29:ALA:HB3	1.91	0.53
1:D:188:TYR:HE2	1:D:257:CYS:HA	1.73	0.53
1:E:148:THR:HB	1:E:167:GLU:HA	1.89	0.53
1:G:163:VAL:HA	1:G:175:ILE:HG12	1.90	0.53
1:K:272:ALA:HB1	1:K:276:GLU:HB2	1.91	0.53
1:E:238:LYS:HA	1:E:238:LYS:HE3	1.90	0.53
1:E:266:PHE:CZ	1:F:282:ILE:HA	2.44	0.53
1:K:100:GLU:HG3	1:K:101:HIS:CD2	2.44	0.53
1:D:43:VAL:CG1	1:F:166:TYR:HB2	2.38	0.53
1:K:359:LYS:HD2	1:K:360:GLN:N	2.24	0.53
1:L:39:ARG:HE	1:M:263:GLN:HG2	1.73	0.53
1:I:216:LEU:HB3	1:I:254:ARG:HG3	1.91	0.53
1:A:7:ALA:HA	1:A:102:PRO:HG2	1.91	0.53
1:F:193:LEU:HB3	1:F:200:PHE:HE1	1.73	0.53
1:F:290:ARG:HD2	1:F:294:TYR:HE2	1.73	0.53
1:I:100:GLU:HG2	1:I:101:HIS:CD2	2.44	0.53
1:I:185:LEU:HD21	1:I:261:LEU:HB2	1.91	0.53
1:A:22:ALA:HB1	1:A:348:SER:HB2	1.91	0.52
1:B:359:LYS:HD2	1:B:360:GLN:N	2.24	0.52
1:D:359:LYS:HD2	1:D:360:GLN:N	2.24	0.52
1:A:243:PRO:O	1:C:322:PRO:C	2.47	0.52
1:D:45:VAL:CG1	1:F:142:LEU:HD13	2.35	0.52
1:J:240:TYR:HB3	1:J:248:ILE:HG22	1.91	0.52
1:J:15:GLY:O	1:J:32:PRO:HA	2.10	0.52
1:A:312:ARG:O	1:A:316:GLU:HB2	2.09	0.52
1:D:45:VAL:CG2	1:F:164:PRO:HA	2.32	0.52
1:K:305:MET:SD	1:K:336:LYS:HB3	2.49	0.52
1:L:9:VAL:HG21	1:L:344:SER:HA	1.92	0.52
1:M:7:ALA:HB3	1:M:22:ALA:HB2	1.92	0.52
1:D:153:LEU:HD21	1:D:274:ILE:HG23	1.91	0.52
1:D:57:GLU:OE1	1:F:291:LYS:HE2	2.02	0.52
1:D:45:VAL:HG22	1:F:165:ILE:H	1.73	0.52
1:I:200:PHE:HA	1:I:205:GLU:HB3	1.91	0.52
1:N:159:VAL:HA	1:N:178:LEU:O	2.10	0.52
1:N:58:ALA:HB1	1:N:65:LEU:HD11	1.91	0.52
1:N:70:PRO:HG2	1:N:71:ILE:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:PRO:HG3	1:E:174:ALA:HB3	1.90	0.52
1:H:39:ARG:HD3	1:H:66:THR:HG23	1.91	0.52
1:C:44:MET:HB2	1:C:47:MET:HB2	1.91	0.52
1:D:42:GLY:HA3	1:F:285:CYS:CB	2.40	0.52
1:F:359:LYS:HD2	1:F:360:GLN:N	2.24	0.52
1:G:162:ASN:O	1:G:175:ILE:HA	2.10	0.52
1:I:61:LYS:HE3	1:K:166:TYR:HE1	1.75	0.52
1:L:296:ASN:HA	1:L:330:ILE:HD11	1.91	0.52
1:C:296:ASN:HA	1:C:330:ILE:HD11	1.91	0.52
1:D:45:VAL:CG1	1:F:165:ILE:HD13	2.39	0.52
1:I:210:ARG:HB3	1:I:210:ARG:CZ	2.39	0.52
1:J:284:LYS:HZ3	1:J:284:LYS:HB2	1.74	0.52
1:A:53:TYR:CE2	1:A:61:LYS:HD2	2.44	0.52
1:B:64:ILE:HG23	1:C:267:ILE:CG1	2.38	0.52
1:A:9:VAL:O	1:A:19:ALA:HA	2.10	0.52
1:F:238:LYS:HE3	1:F:238:LYS:HA	1.92	0.52
1:G:106:THR:HG21	1:G:339:VAL:HG12	1.92	0.52
1:G:8:LEU:HG	1:G:101:HIS:HB3	1.92	0.52
1:L:40:HIS:HE1	1:M:263:GLN:O	1.93	0.52
1:A:261:LEU:HG	1:A:274:ILE:HG13	1.92	0.52
1:A:53:TYR:HD2	1:A:57:GLU:HB3	1.75	0.52
1:A:65:LEU:HB2	1:B:267:ILE:HD12	1.92	0.52
1:C:213:LYS:HA	1:C:217:CYS:SG	2.50	0.52
1:C:265:SER:OG	1:C:270:GLU:HA	2.10	0.52
1:B:105:LEU:O	1:B:134:VAL:HA	2.10	0.51
1:D:19:ALA:HB3	1:D:29:ALA:HB3	1.91	0.51
1:I:162:ASN:O	1:I:175:ILE:HA	2.10	0.51
1:K:359:LYS:HD2	1:K:360:GLN:HB2	1.91	0.51
1:N:355:MET:HA	1:N:373:LYS:HD3	1.92	0.51
1:A:104:LEU:HA	1:A:133:TYR:O	2.10	0.51
1:A:53:TYR:CD2	1:A:57:GLU:HB3	2.45	0.51
1:D:286:ASP:HB3	1:D:289:ILE:HG23	1.91	0.51
1:E:201:VAL:HG12	1:E:202:THR:HG23	1.93	0.51
1:K:15:GLY:O	1:K:32:PRO:HA	2.09	0.51
1:N:359:LYS:HD2	1:N:360:GLN:N	2.25	0.51
1:A:153:LEU:HD11	1:A:274:ILE:HD13	1.91	0.51
1:D:197:GLY:CA	1:E:112:PRO:HA	2.40	0.51
1:J:204:ALA:HA	1:J:207:GLU:HB2	1.92	0.51
1:D:45:VAL:HG22	1:F:165:ILE:N	2.26	0.51
1:I:194:THR:HB	1:J:110:LEU:HB3	1.93	0.51
1:A:136:ILE:H	1:A:136:ILE:HD12	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ASN:OD1	1:C:277:THR:HG23	2.11	0.51
1:D:68:LYS:O	1:D:70:PRO:HD3	2.10	0.51
1:H:182:GLY:HA2	1:H:303:THR:OG1	2.11	0.51
1:H:359:LYS:HD2	1:H:360:GLN:N	2.26	0.51
1:K:192:ILE:HA	1:L:112:PRO:CG	2.34	0.51
1:B:349:LEU:HB3	1:B:352:PHE:HB2	1.91	0.51
1:D:238:LYS:HA	1:D:238:LYS:HE3	1.92	0.51
1:J:174:ALA:HA	1:J:284:LYS:HZ3	1.76	0.51
1:N:137:GLN:HG2	1:N:339:VAL:HG11	1.93	0.51
1:A:212:ILE:HG23	1:A:216:LEU:HD12	1.92	0.51
1:E:206:ARG:NH1	1:F:271:SER:O	2.43	0.51
1:N:294:TYR:HE1	1:N:321:ALA:HB1	1.75	0.51
1:D:45:VAL:HG13	1:F:165:ILE:HD12	1.92	0.51
1:D:48:GLY:C	1:F:166:TYR:CD2	2.84	0.51
1:F:191:LYS:HB3	1:G:173:HIS:HB2	1.93	0.51
1:H:11:ASP:O	1:H:17:VAL:HA	2.11	0.51
1:I:153:LEU:HD23	1:I:299:MET:HG2	1.92	0.51
1:I:160:THR:HB	1:I:178:LEU:HB3	1.93	0.51
1:A:359:LYS:HD2	1:A:360:GLN:HB2	1.92	0.51
1:E:160:THR:O	1:E:177:ARG:HA	2.11	0.51
1:D:45:VAL:CG1	1:F:165:ILE:HD12	2.40	0.51
1:D:49:GLN:HA	1:F:166:TYR:CZ	2.46	0.51
1:G:34:ILE:O	1:G:54:VAL:HA	2.11	0.51
1:I:163:VAL:HG22	1:I:175:ILE:HG23	1.93	0.51
1:L:359:LYS:HD2	1:L:360:GLN:HB2	1.93	0.51
1:B:357:ILE:HG13	1:B:370:VAL:HG22	1.93	0.51
1:E:359:LYS:HD2	1:E:360:GLN:HB2	1.93	0.51
1:A:238:LYS:HE3	1:A:238:LYS:HA	1.92	0.50
1:J:163:VAL:HG22	1:J:175:ILE:HG23	1.92	0.50
1:K:244:ASP:HB2	1:M:290:ARG:HB2	1.92	0.50
1:M:19:ALA:HB3	1:M:29:ALA:HB3	1.93	0.50
1:E:99:GLU:HB3	1:E:128:ASN:ND2	2.26	0.50
1:M:359:LYS:HD2	1:M:360:GLN:N	2.26	0.50
1:B:174:ALA:HB2	1:B:285:CYS:SG	2.51	0.50
1:L:322:PRO:O	1:L:325:MET:HG2	2.10	0.50
1:D:210:ARG:O	1:D:213:LYS:HB3	2.11	0.50
1:D:182:GLY:HA2	1:D:303:THR:OG1	2.11	0.50
1:D:61:LYS:NZ	1:F:291:LYS:CG	2.72	0.50
1:F:212:ILE:HG23	1:F:216:LEU:HD12	1.93	0.50
1:H:328:LYS:HZ1	1:H:330:ILE:HG13	1.76	0.50
1:E:106:THR:HG22	1:E:140:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:359:LYS:HD2	1:E:360:GLN:N	2.27	0.50
1:H:210:ARG:HH11	1:H:210:ARG:HB2	1.77	0.50
1:I:139:VAL:HA	1:I:165:ILE:HD13	1.93	0.50
1:D:64:ILE:HG12	1:F:285:CYS:O	2.11	0.50
1:F:45:VAL:HG22	1:H:166:TYR:CE1	2.27	0.50
1:D:305:MET:SD	1:D:336:LYS:HB3	2.51	0.50
1:F:193:LEU:HG	1:F:250:ILE:HD12	1.93	0.50
1:I:305:MET:SD	1:I:336:LYS:HB3	2.51	0.50
1:J:100:GLU:HG2	1:J:101:HIS:CD2	2.46	0.50
1:J:10:CYS:HA	1:J:18:LYS:O	2.12	0.50
1:J:332:PRO:HB2	1:J:335:ARG:HB3	1.92	0.50
1:K:162:ASN:HB2	1:K:176:MET:HB2	1.93	0.50
1:A:153:LEU:HD13	1:A:162:ASN:ND2	2.27	0.50
1:E:120:THR:HG21	1:E:370:VAL:HG21	1.94	0.50
1:F:174:ALA:HB2	1:F:284:LYS:HG2	1.93	0.50
1:G:267:ILE:HD13	1:H:169:TYR:OH	2.11	0.50
1:N:102:PRO:HD3	1:N:130:PRO:HG2	1.93	0.50
1:E:34:ILE:O	1:E:54:VAL:HA	2.12	0.50
1:G:166:TYR:HB2	1:G:289:ILE:HD13	1.94	0.50
1:M:37:ARG:HB3	1:M:38:PRO:CD	2.42	0.50
1:C:203:THR:HG22	1:C:206:ARG:NH2	2.27	0.49
1:G:151:ILE:HB	1:G:293:LEU:HG	1.94	0.49
1:L:292:ASP:HB3	1:L:296:ASN:HD22	1.76	0.49
1:L:312:ARG:HD2	1:L:315:LYS:HE3	1.94	0.49
1:E:213:LYS:HG3	1:E:306:TYR:OH	2.12	0.49
1:H:102:PRO:HB3	1:H:131:ALA:HB3	1.94	0.49
1:N:109:PRO:HA	1:N:136:ILE:HG23	1.93	0.49
1:B:11:ASP:HB3	1:B:18:LYS:HB2	1.95	0.49
1:C:359:LYS:HD2	1:C:360:GLN:HB2	1.93	0.49
1:D:64:ILE:H	1:F:287:ILE:HD13	1.75	0.49
1:H:36:GLY:HA3	1:H:65:LEU:HD13	1.93	0.49
1:J:263:GLN:HE21	1:J:263:GLN:HA	1.76	0.49
1:K:193:LEU:HB3	1:K:198:TYR:HB2	1.93	0.49
1:L:10:CYS:HA	1:L:18:LYS:O	2.12	0.49
1:M:283:MET:SD	1:M:290:ARG:NH2	2.85	0.49
1:I:104:LEU:HA	1:I:133:TYR:O	2.12	0.49
1:J:243:PRO:HD2	1:L:291:LYS:HD3	1.95	0.49
1:B:8:LEU:HA	1:B:21:PHE:HA	1.94	0.49
1:G:242:LEU:HD13	1:G:248:ILE:HD11	1.93	0.49
1:I:239:SER:HA	1:I:248:ILE:O	2.13	0.49
1:J:153:LEU:HD21	1:J:274:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:212:ILE:HG23	1:L:216:LEU:HD12	1.95	0.49
1:L:242:LEU:HD11	1:L:248:ILE:HD13	1.93	0.49
1:L:193:LEU:HG	1:L:250:ILE:HD11	1.94	0.49
1:N:7:ALA:HA	1:N:102:PRO:HG2	1.94	0.49
1:N:282:ILE:HG22	1:N:290:ARG:HD2	1.94	0.49
1:B:19:ALA:HB3	1:B:29:ALA:HB3	1.95	0.49
1:D:43:VAL:CG1	1:F:169:TYR:CD1	2.91	0.49
1:D:44:MET:CG	1:F:293:LEU:HD11	2.39	0.49
1:L:210:ARG:O	1:L:213:LYS:HB3	2.12	0.49
1:A:10:CYS:HA	1:A:18:LYS:O	2.12	0.49
1:A:117:GLU:HB3	1:A:367:PRO:HB3	1.94	0.49
1:B:15:GLY:O	1:B:32:PRO:HA	2.12	0.49
1:E:200:PHE:H	1:F:180:LEU:HD22	1.77	0.49
1:K:195:GLU:HB2	1:L:112:PRO:CB	2.42	0.49
1:E:109:PRO:HA	1:E:136:ILE:HG23	1.93	0.49
1:G:278:THR:HG21	1:G:297:ASN:OD1	2.12	0.49
1:F:46:GLY:N	1:H:167:GLU:CG	2.76	0.49
1:I:252:ASN:HA	1:I:255:PHE:HE2	1.76	0.49
1:L:106:THR:HG22	1:L:140:LEU:HD12	1.95	0.49
1:L:204:ALA:HB1	1:N:287:ILE:HG23	1.94	0.49
1:N:299:MET:O	1:N:332:PRO:HD2	2.13	0.49
1:A:86:TRP:HH2	1:A:119:MET:HG2	1.78	0.49
1:B:205:GLU:O	1:B:208:ILE:HG12	2.13	0.49
1:D:240:TYR:HB3	1:D:248:ILE:HB	1.94	0.49
1:D:61:LYS:HZ3	1:F:291:LYS:CD	2.06	0.49
1:J:102:PRO:HA	1:J:131:ALA:O	2.12	0.49
1:K:203:THR:O	1:K:207:GLU:HB2	2.12	0.49
1:A:264:PRO:HD3	1:A:273:GLY:HA3	1.95	0.49
1:E:22:ALA:HB1	1:E:348:SER:HB2	1.95	0.49
1:F:290:ARG:HD2	1:F:294:TYR:CE2	2.48	0.49
1:I:155:SER:HA	1:I:160:THR:HA	1.94	0.49
1:K:217:CYS:HA	1:K:254:ARG:O	2.13	0.49
1:C:8:LEU:HG	1:C:101:HIS:HB3	1.94	0.48
1:F:74:GLY:O	1:F:108:ALA:HB2	2.12	0.48
1:G:186:THR:HG21	1:G:210:ARG:HG2	1.94	0.48
1:M:238:LYS:HE3	1:M:238:LYS:HA	1.95	0.48
1:N:242:LEU:HD22	1:N:246:GLN:HB3	1.94	0.48
1:N:59:GLN:OE1	1:N:62:ARG:NH1	2.46	0.48
1:B:64:ILE:HG23	1:C:267:ILE:HB	0.69	0.48
1:C:153:LEU:HD21	1:C:274:ILE:HG23	1.96	0.48
1:F:10:CYS:HA	1:F:18:LYS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:153:LEU:HA	1:L:161:HIS:O	2.13	0.48
1:M:114:ALA:HA	1:M:117:GLU:HB2	1.96	0.48
1:N:104:LEU:HG	1:N:133:TYR:HB3	1.94	0.48
1:N:140:LEU:O	1:N:342:GLY:HA3	2.13	0.48
1:B:137:GLN:HA	1:B:339:VAL:HG13	1.95	0.48
1:B:60:SER:OG	1:D:287:ILE:CD1	2.61	0.48
1:E:191:LYS:HA	1:E:194:THR:OG1	2.13	0.48
1:I:106:THR:HG22	1:I:140:LEU:HD12	1.95	0.48
1:I:189:LEU:HD13	1:I:257:CYS:SG	2.53	0.48
1:L:162:ASN:O	1:L:175:ILE:HA	2.13	0.48
1:L:299:MET:O	1:L:332:PRO:HD2	2.12	0.48
1:A:239:SER:HA	1:A:248:ILE:O	2.13	0.48
1:E:195:GLU:HA	1:F:177:ARG:HB3	1.96	0.48
1:B:43:VAL:HB	1:D:169:TYR:OH	2.13	0.48
1:D:162:ASN:O	1:D:175:ILE:HA	2.14	0.48
1:D:106:THR:HG21	1:D:339:VAL:HG12	1.96	0.48
1:G:32:PRO:HB2	1:G:34:ILE:HG12	1.94	0.48
1:K:162:ASN:O	1:K:175:ILE:HA	2.13	0.48
1:A:359:LYS:HD2	1:A:360:GLN:N	2.28	0.48
1:J:262:PHE:O	1:J:275:HIS:HE1	1.97	0.48
1:A:53:TYR:CZ	1:A:61:LYS:HD3	2.47	0.48
1:B:189:LEU:HD12	1:B:192:ILE:HD11	1.96	0.48
1:F:119:MET:O	1:F:123:MET:HG2	2.13	0.48
1:F:61:LYS:O	1:F:65:LEU:HG	2.14	0.48
1:G:12:ASN:HA	1:G:17:VAL:HG22	1.95	0.48
1:J:102:PRO:HB3	1:J:131:ALA:HB3	1.96	0.48
1:M:155:SER:HA	1:M:160:THR:HA	1.95	0.48
1:B:286:ASP:O	1:B:289:ILE:HG13	2.14	0.48
1:I:359:LYS:HD2	1:I:360:GLN:HB2	1.95	0.48
1:J:182:GLY:O	1:J:213:LYS:NZ	2.44	0.48
1:A:330:ILE:O	1:A:332:PRO:HD3	2.13	0.48
1:B:64:ILE:N	1:C:267:ILE:HA	2.29	0.48
1:B:62:ARG:HG2	1:C:268:GLY:HA2	1.96	0.48
1:D:45:VAL:HG11	1:F:165:ILE:HD13	1.95	0.48
1:E:191:LYS:O	1:F:176:MET:SD	2.72	0.48
1:I:238:LYS:O	1:I:249:THR:HA	2.14	0.48
1:J:10:CYS:HB3	1:J:105:LEU:HD23	1.96	0.48
1:J:205:GLU:HB2	1:L:286:ASP:HB3	1.96	0.48
1:M:164:PRO:HG3	1:M:174:ALA:HB3	1.96	0.48
1:L:39:ARG:NH2	1:M:264:PRO:HD2	2.29	0.48
1:G:267:ILE:HD11	1:H:169:TYR:OH	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:151:ILE:HD11	1:J:162:ASN:HB3	1.95	0.48
1:K:252:ASN:O	1:K:256:ARG:NH2	2.47	0.48
1:L:253:GLU:HA	1:L:256:ARG:HE	1.78	0.48
1:B:155:SER:HA	1:B:160:THR:HA	1.96	0.47
1:D:164:PRO:HG3	1:D:285:CYS:SG	2.54	0.47
1:D:57:GLU:OE2	1:F:291:LYS:CD	2.61	0.47
1:E:152:VAL:HA	1:E:298:VAL:HB	1.96	0.47
1:G:332:PRO:HB2	1:G:335:ARG:HB3	1.96	0.47
1:H:10:CYS:SG	1:H:89:THR:HG21	2.53	0.47
1:J:292:ASP:O	1:J:296:ASN:HB2	2.14	0.47
1:M:162:ASN:O	1:M:175:ILE:HA	2.14	0.47
1:N:152:VAL:O	1:N:162:ASN:HA	2.14	0.47
1:A:15:GLY:O	1:A:32:PRO:HA	2.14	0.47
1:B:11:ASP:O	1:B:17:VAL:HA	2.14	0.47
1:B:39:ARG:CD	1:B:66:THR:HG23	2.37	0.47
1:D:11:ASP:O	1:D:17:VAL:HA	2.14	0.47
1:D:197:GLY:HA3	1:D:198:TYR:HA	1.67	0.47
1:D:45:VAL:CG1	1:F:142:LEU:CD1	2.92	0.47
1:G:103:THR:O	1:G:132:MET:HA	2.13	0.47
1:J:44:MET:HB2	1:J:47:MET:HB2	1.97	0.47
1:K:152:VAL:O	1:K:162:ASN:HA	2.14	0.47
1:K:188:TYR:HA	1:K:191:LYS:HD3	1.95	0.47
1:L:39:ARG:HH21	1:M:264:PRO:HD2	1.79	0.47
1:A:135:ALA:HB3	1:A:140:LEU:HD11	1.97	0.47
1:B:250:ILE:HG23	1:B:253:GLU:HB2	1.96	0.47
1:D:298:VAL:HA	1:D:330:ILE:O	2.14	0.47
1:I:105:LEU:O	1:I:134:VAL:HA	2.14	0.47
1:N:9:VAL:HG21	1:N:344:SER:HA	1.97	0.47
1:D:15:GLY:O	1:D:32:PRO:HA	2.14	0.47
1:F:9:VAL:HG13	1:F:104:LEU:HD22	1.96	0.47
1:G:86:TRP:HH2	1:G:119:MET:HG3	1.79	0.47
1:K:11:ASP:HA	1:K:106:THR:OG1	2.15	0.47
1:K:198:TYR:CZ	1:K:248:ILE:HG13	2.48	0.47
1:L:359:LYS:HD2	1:L:360:GLN:N	2.28	0.47
1:E:62:ARG:HE	1:E:67:LEU:HD11	1.78	0.47
1:H:36:GLY:HA2	1:H:66:THR:O	2.15	0.47
1:H:99:GLU:HA	1:H:130:PRO:HD3	1.96	0.47
1:I:10:CYS:HA	1:I:18:LYS:O	2.15	0.47
1:I:118:LYS:NZ	1:I:121:GLN:OE1	2.47	0.47
1:J:8:LEU:HG	1:J:101:HIS:HB3	1.95	0.47
1:K:58:ALA:O	1:K:62:ARG:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:8:LEU:HG	1:L:101:HIS:HB3	1.96	0.47
1:M:152:VAL:O	1:M:162:ASN:HA	2.14	0.47
1:D:251:GLY:O	1:D:254:ARG:HG3	2.15	0.47
1:L:9:VAL:O	1:L:19:ALA:HA	2.15	0.47
1:D:200:PHE:HZ	1:D:248:ILE:HG12	1.79	0.47
1:E:287:ILE:HA	1:E:290:ARG:HB2	1.95	0.47
1:F:201:VAL:HG21	1:G:177:ARG:HD3	1.95	0.47
1:G:45:VAL:HG23	1:I:167:GLU:HB3	1.96	0.47
1:H:186:THR:OG1	1:H:213:LYS:HD2	2.14	0.47
1:I:186:THR:HG23	1:I:213:LYS:HB2	1.94	0.47
1:L:304:THR:HA	1:L:309:ILE:HD13	1.95	0.47
1:L:63:GLY:O	1:M:270:GLU:HB2	2.15	0.47
1:N:71:ILE:HA	1:N:76:ILE:HA	1.96	0.47
1:A:286:ASP:O	1:A:290:ARG:HG3	2.15	0.47
1:E:86:TRP:CH2	1:E:119:MET:HG3	2.50	0.47
1:D:64:ILE:CG1	1:F:286:ASP:HA	2.44	0.47
1:I:109:PRO:HA	1:I:136:ILE:HG23	1.97	0.47
1:N:105:LEU:O	1:N:134:VAL:HA	2.15	0.47
1:D:62:ARG:HG3	1:D:67:LEU:HD21	1.95	0.47
1:C:32:PRO:HG2	1:C:55:GLY:HA2	1.97	0.47
1:D:39:ARG:NH2	1:E:264:PRO:O	2.48	0.47
1:I:252:ASN:OD1	1:J:113:LYS:NZ	2.47	0.47
1:K:213:LYS:HA	1:K:217:CYS:SG	2.54	0.47
1:K:147:ARG:NH1	1:K:296:ASN:OD1	2.46	0.47
1:A:62:ARG:CD	1:C:287:ILE:HD11	2.34	0.47
1:F:136:ILE:H	1:F:136:ILE:HD12	1.80	0.47
1:F:369:ILE:O	1:F:373:LYS:HB2	2.14	0.47
1:G:19:ALA:HB3	1:G:29:ALA:HB3	1.96	0.47
1:G:263:GLN:HA	1:G:263:GLN:HE21	1.79	0.47
1:G:32:PRO:HG2	1:G:55:GLY:HA2	1.97	0.47
1:G:45:VAL:HG21	1:I:167:GLU:OE1	2.14	0.47
1:J:359:LYS:HD2	1:J:360:GLN:N	2.29	0.47
1:K:239:SER:HA	1:K:248:ILE:O	2.15	0.47
1:K:153:LEU:HD23	1:K:299:MET:HG2	1.96	0.47
1:L:192:ILE:HA	1:L:195:GLU:HB2	1.96	0.47
1:M:86:TRP:CH2	1:M:119:MET:HG3	2.49	0.47
1:A:162:ASN:OD1	1:A:277:THR:HG23	2.16	0.46
1:F:142:LEU:HD22	1:F:165:ILE:HD13	1.97	0.46
1:F:153:LEU:HA	1:F:161:HIS:O	2.15	0.46
1:H:36:GLY:O	1:H:52:SER:HA	2.15	0.46
1:K:188:TYR:CE2	1:K:257:CYS:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:242:LEU:HD22	1:K:242:LEU:H	1.80	0.46
1:K:242:LEU:O	1:K:244:ASP:N	2.48	0.46
1:A:147:ARG:NH1	1:A:296:ASN:OD1	2.48	0.46
1:A:198:TYR:OH	1:A:248:ILE:HA	2.14	0.46
1:B:148:THR:HB	1:B:167:GLU:HA	1.98	0.46
1:E:9:VAL:HA	1:E:104:LEU:O	2.15	0.46
1:I:36:GLY:HA3	1:I:65:LEU:HD13	1.96	0.46
1:J:190:MET:HG3	1:J:200:PHE:CD1	2.50	0.46
1:E:206:ARG:HB2	1:F:265:SER:HA	1.98	0.46
1:F:152:VAL:O	1:F:162:ASN:HA	2.16	0.46
1:L:109:PRO:HA	1:L:136:ILE:HG23	1.96	0.46
1:L:353:GLN:HA	1:L:356:TRP:CD1	2.50	0.46
1:M:37:ARG:HB3	1:M:38:PRO:HD2	1.97	0.46
1:D:193:LEU:HB3	1:D:198:TYR:HB2	1.97	0.46
1:D:32:PRO:O	1:D:55:GLY:HA2	2.15	0.46
1:F:102:PRO:HB3	1:F:131:ALA:HB3	1.97	0.46
1:G:155:SER:HA	1:G:160:THR:HA	1.96	0.46
1:H:153:LEU:HD12	1:H:161:HIS:O	2.14	0.46
1:I:359:LYS:HD2	1:I:360:GLN:N	2.30	0.46
1:L:11:ASP:HA	1:L:106:THR:OG1	2.15	0.46
1:C:119:MET:O	1:C:123:MET:HG2	2.15	0.46
1:F:182:GLY:O	1:F:213:LYS:NZ	2.48	0.46
1:E:266:PHE:CE1	1:F:282:ILE:HA	2.51	0.46
1:M:104:LEU:HA	1:M:133:TYR:O	2.16	0.46
1:D:104:LEU:HG	1:D:133:TYR:HB3	1.97	0.46
1:D:65:LEU:HG	1:F:287:ILE:HG21	1.98	0.46
1:H:139:VAL:HG22	1:H:170:ALA:HB2	1.97	0.46
1:J:219:VAL:HG22	1:J:258:PRO:HB3	1.97	0.46
1:B:283:MET:SD	1:B:290:ARG:NH2	2.89	0.46
1:C:162:ASN:HB2	1:C:176:MET:HB2	1.98	0.46
1:D:212:ILE:HG23	1:D:216:LEU:HD12	1.98	0.46
1:D:58:ALA:HB1	1:D:65:LEU:HD11	1.97	0.46
1:E:207:GLU:HB3	1:F:269:MET:N	2.31	0.46
1:F:11:ASP:HA	1:F:106:THR:OG1	2.16	0.46
1:D:49:GLN:N	1:F:166:TYR:CE2	2.84	0.46
1:G:330:ILE:O	1:G:332:PRO:HD3	2.15	0.46
1:L:186:THR:HG21	1:L:210:ARG:HG2	1.98	0.46
1:M:174:ALA:HB1	1:M:281:SER:O	2.15	0.46
1:B:209:VAL:HA	1:B:212:ILE:HD12	1.97	0.46
1:D:61:LYS:NZ	1:F:291:LYS:CB	2.76	0.46
1:G:196:ARG:NH2	1:G:249:THR:OG1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:286:ASP:O	1:J:290:ARG:HG3	2.16	0.46
1:J:305:MET:SD	1:J:336:LYS:HB3	2.56	0.46
1:K:195:GLU:H	1:L:112:PRO:HD2	1.81	0.46
1:C:106:THR:HG22	1:C:140:LEU:HD12	1.98	0.46
1:E:267:ILE:HB	1:F:287:ILE:O	2.16	0.46
1:H:155:SER:HA	1:H:160:THR:HA	1.96	0.46
1:I:192:ILE:HB	1:I:253:GLU:HG3	1.97	0.46
1:B:286:ASP:O	1:B:290:ARG:HG2	2.15	0.46
1:B:124:PHE:HE1	1:B:359:LYS:HA	1.80	0.46
1:C:162:ASN:O	1:C:175:ILE:HA	2.16	0.46
1:E:268:GLY:H	1:F:290:ARG:NE	2.13	0.46
1:D:61:LYS:CE	1:F:291:LYS:HB3	2.46	0.46
1:J:119:MET:O	1:J:123:MET:HG2	2.16	0.46
1:B:359:LYS:HD2	1:B:360:GLN:HB2	1.98	0.45
1:D:197:GLY:HA2	1:E:113:LYS:N	2.31	0.45
1:G:359:LYS:HD2	1:G:360:GLN:N	2.31	0.45
1:I:220:ALA:O	1:I:312:ARG:HD3	2.15	0.45
1:K:9:VAL:HA	1:K:104:LEU:O	2.16	0.45
1:N:210:ARG:CZ	1:N:210:ARG:HB3	2.46	0.45
1:N:9:VAL:O	1:N:19:ALA:HA	2.16	0.45
1:A:100:GLU:HG3	1:A:101:HIS:CD2	2.51	0.45
1:B:36:GLY:HA2	1:B:66:THR:O	2.16	0.45
1:D:186:THR:HG21	1:D:210:ARG:HG2	1.98	0.45
1:D:8:LEU:HG	1:D:101:HIS:HB3	1.98	0.45
1:F:17:VAL:O	1:F:30:VAL:HA	2.16	0.45
1:F:189:LEU:HD13	1:F:257:CYS:SG	2.55	0.45
1:J:73:HIS:HB3	1:J:177:ARG:NH1	2.32	0.45
1:N:162:ASN:O	1:N:175:ILE:HA	2.16	0.45
1:J:303:THR:HG23	1:J:306:TYR:CE2	2.51	0.45
1:K:238:LYS:HE3	1:K:238:LYS:HA	1.98	0.45
1:K:9:VAL:HG21	1:K:344:SER:HA	1.98	0.45
1:K:71:ILE:HA	1:K:76:ILE:HA	1.99	0.45
1:M:153:LEU:HA	1:M:161:HIS:O	2.17	0.45
1:M:37:ARG:HG3	1:M:51:ASP:O	2.17	0.45
1:M:7:ALA:HA	1:M:102:PRO:HG2	1.99	0.45
1:N:133:TYR:CE1	1:N:135:ALA:HB2	2.51	0.45
1:N:62:ARG:HA	1:N:65:LEU:HB3	1.98	0.45
1:B:108:ALA:HB3	1:B:111:ASN:HD22	1.81	0.45
1:H:238:LYS:HE3	1:H:238:LYS:HA	1.99	0.45
1:H:263:GLN:HE21	1:H:263:GLN:HA	1.81	0.45
1:J:11:ASP:HA	1:J:106:THR:OG1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:11:ASP:O	1:M:17:VAL:HA	2.16	0.45
1:M:65:LEU:HG	1:N:269:MET:HA	1.98	0.45
1:N:324:THR:HB	1:N:325:MET:SD	2.57	0.45
1:B:102:PRO:HD3	1:B:130:PRO:HG2	1.98	0.45
1:B:111:ASN:OD1	1:B:115:ASN:HB3	2.16	0.45
1:B:163:VAL:HG13	1:B:175:ILE:HG12	1.98	0.45
1:D:263:GLN:HA	1:D:263:GLN:HE21	1.81	0.45
1:E:62:ARG:HB2	1:E:62:ARG:NH2	2.30	0.45
1:F:227:MET:HB2	1:F:255:PHE:HE1	1.82	0.45
1:C:118:LYS:NZ	1:C:121:GLN:OE1	2.48	0.45
1:D:210:ARG:HB3	1:D:210:ARG:CZ	2.46	0.45
1:D:65:LEU:CG	1:F:287:ILE:HG21	2.47	0.45
1:I:64:ILE:HG13	1:I:65:LEU:HG	1.98	0.45
1:M:135:ALA:HB3	1:M:140:LEU:HD11	1.99	0.45
1:A:105:LEU:O	1:A:134:VAL:HA	2.17	0.45
1:B:154:ASP:O	1:B:160:THR:HA	2.16	0.45
1:L:118:LYS:NZ	1:L:121:GLN:OE1	2.48	0.45
1:N:38:PRO:HB2	1:N:40:HIS:O	2.17	0.45
1:A:11:ASP:O	1:A:17:VAL:HA	2.17	0.45
1:A:305:MET:SD	1:A:336:LYS:HB3	2.57	0.45
1:B:136:ILE:HB	1:B:139:VAL:HG23	1.99	0.45
1:B:200:PHE:O	1:B:206:ARG:HG3	2.16	0.45
1:C:165:ILE:HA	1:C:170:ALA:HA	1.99	0.45
1:D:42:GLY:HA3	1:F:285:CYS:HB2	1.98	0.45
1:F:219:VAL:HG21	1:F:309:ILE:HB	1.98	0.45
1:I:7:ALA:HA	1:I:102:PRO:HG2	1.98	0.45
1:K:105:LEU:O	1:K:134:VAL:HA	2.17	0.45
1:K:240:TYR:O	1:K:248:ILE:HG22	2.16	0.45
1:C:100:GLU:HG2	1:C:101:HIS:CD2	2.52	0.45
1:C:291:LYS:HZ3	1:C:292:ASP:CG	2.19	0.45
1:E:7:ALA:HA	1:E:102:PRO:HG2	1.98	0.45
1:L:198:TYR:OH	1:L:248:ILE:HA	2.17	0.45
1:L:180:LEU:HD21	1:L:264:PRO:HB3	1.99	0.45
1:N:162:ASN:OD1	1:N:176:MET:HB3	2.16	0.45
1:M:39:ARG:HB2	1:N:265:SER:C	2.36	0.45
1:E:9:VAL:O	1:E:19:ALA:HA	2.17	0.45
1:I:294:TYR:O	1:I:327:ILE:HA	2.15	0.45
1:L:262:PHE:O	1:L:275:HIS:HE1	1.99	0.45
1:K:243:PRO:HB3	1:M:291:LYS:HE3	1.98	0.45
1:A:113:LYS:O	1:A:116:ARG:HB3	2.17	0.44
1:A:220:ALA:O	1:A:312:ARG:NH2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:HIS:HA	1:B:102:PRO:HD2	1.85	0.44
1:D:17:VAL:HG23	1:D:33:SER:OG	2.18	0.44
1:F:153:LEU:HD21	1:F:274:ILE:HG23	1.99	0.44
1:I:8:LEU:HG	1:I:101:HIS:HB3	1.98	0.44
1:L:193:LEU:O	1:L:196:ARG:HB3	2.17	0.44
1:M:118:LYS:NZ	1:M:121:GLN:OE1	2.48	0.44
1:B:104:LEU:HA	1:B:133:TYR:O	2.17	0.44
1:C:10:CYS:HB3	1:C:105:LEU:HD23	1.99	0.44
1:D:182:GLY:O	1:D:213:LYS:NZ	2.50	0.44
1:D:188:TYR:CE2	1:D:257:CYS:HA	2.51	0.44
1:F:59:GLN:O	1:F:62:ARG:HD2	2.17	0.44
1:K:243:PRO:O	1:M:291:LYS:HG2	2.16	0.44
1:M:171:LEU:HA	1:M:172:PRO:HD3	1.71	0.44
1:M:163:VAL:HG22	1:M:175:ILE:HG23	2.00	0.44
1:N:230:ALA:HB1	1:N:252:ASN:HD22	1.82	0.44
1:B:17:VAL:C	1:B:18:LYS:HE3	2.38	0.44
1:J:104:LEU:HG	1:J:133:TYR:HB3	1.99	0.44
1:L:10:CYS:HB3	1:L:105:LEU:HD23	2.00	0.44
1:K:243:PRO:HB2	1:M:288:ASP:O	2.17	0.44
1:D:10:CYS:HB3	1:D:105:LEU:HD23	1.99	0.44
1:D:328:LYS:HZ1	1:D:330:ILE:HG13	1.81	0.44
1:D:44:MET:O	1:F:165:ILE:O	2.35	0.44
1:M:147:ARG:NH1	1:M:296:ASN:OD1	2.51	0.44
1:N:321:ALA:HA	1:N:322:PRO:HD2	1.67	0.44
1:C:196:ARG:NH2	1:C:249:THR:OG1	2.51	0.44
1:D:194:THR:HA	1:D:197:GLY:C	2.38	0.44
1:D:35:VAL:HG22	1:D:54:VAL:HG22	1.98	0.44
1:E:312:ARG:HD2	1:E:315:LYS:HE3	1.99	0.44
1:F:282:ILE:HG22	1:F:283:MET:N	2.33	0.44
1:F:45:VAL:CG1	1:H:167:GLU:HG3	2.47	0.44
1:M:162:ASN:HB2	1:M:176:MET:HB3	1.97	0.44
1:A:193:LEU:HB3	1:A:200:PHE:HE1	1.82	0.44
1:D:37:ARG:HA	1:D:38:PRO:HD2	1.80	0.44
1:D:63:GLY:H	1:E:267:ILE:HA	1.82	0.44
1:E:38:PRO:HD2	1:E:51:ASP:O	2.17	0.44
1:H:212:ILE:HG23	1:H:216:LEU:HD12	1.99	0.44
1:K:186:THR:HG21	1:K:210:ARG:HG2	2.00	0.44
1:L:111:ASN:OD1	1:L:115:ASN:HB3	2.18	0.44
1:A:244:ASP:HA	1:C:323:SER:HB2	1.99	0.44
1:D:44:MET:SD	1:D:45:VAL:HG23	2.58	0.44
1:F:219:VAL:HG22	1:F:258:PRO:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:194:THR:HG22	1:I:198:TYR:O	2.18	0.44
1:J:219:VAL:HG22	1:J:258:PRO:CB	2.48	0.44
1:A:154:ASP:O	1:A:160:THR:HA	2.18	0.44
1:B:135:ALA:HB3	1:B:140:LEU:HD11	1.98	0.44
1:C:163:VAL:HG13	1:C:175:ILE:HG12	2.00	0.44
1:C:366:GLY:O	1:C:369:ILE:HG22	2.18	0.44
1:E:287:ILE:N	1:E:287:ILE:HD12	2.30	0.44
1:F:103:THR:O	1:F:132:MET:HA	2.18	0.44
1:H:53:TYR:CD1	1:H:65:LEU:HD21	2.53	0.44
1:J:112:PRO:HG2	1:J:116:ARG:HB2	2.00	0.44
1:L:217:CYS:O	1:L:307:PRO:HD2	2.18	0.44
1:B:10:CYS:HA	1:B:18:LYS:O	2.18	0.44
1:D:147:ARG:CZ	1:D:330:ILE:HG12	2.48	0.44
1:D:202:THR:H	1:D:205:GLU:HB2	1.82	0.44
1:D:230:ALA:HB1	1:D:252:ASN:HB3	1.99	0.44
1:D:49:GLN:HA	1:F:166:TYR:CE2	2.53	0.44
1:E:219:VAL:HG22	1:E:258:PRO:HB2	1.99	0.44
1:F:50:LYS:NZ	1:F:52:SER:O	2.49	0.44
1:H:155:SER:HB3	1:H:304:THR:HG23	1.99	0.44
1:F:45:VAL:CB	1:H:166:TYR:HE1	2.26	0.44
1:K:193:LEU:O	1:K:196:ARG:HB3	2.17	0.44
1:A:133:TYR:HE2	1:A:374:CYS:HG	1.62	0.43
1:C:359:LYS:HD2	1:C:360:GLN:N	2.33	0.43
1:D:171:LEU:HA	1:D:172:PRO:HD2	1.83	0.43
1:H:262:PHE:HE2	1:H:309:ILE:HG13	1.82	0.43
1:I:45:VAL:HB	1:K:168:GLY:HA3	2.00	0.43
1:K:256:ARG:HD3	1:L:113:LYS:NZ	2.33	0.43
1:N:124:PHE:HE1	1:N:359:LYS:HA	1.83	0.43
1:N:86:TRP:CH2	1:N:119:MET:HG3	2.53	0.43
1:H:9:VAL:HG13	1:H:104:LEU:HD22	2.00	0.43
1:H:118:LYS:NZ	1:H:121:GLN:OE1	2.49	0.43
1:H:53:TYR:HD1	1:H:65:LEU:HD21	1.83	0.43
1:H:7:ALA:HA	1:H:102:PRO:HG2	2.00	0.43
1:K:189:LEU:HD12	1:K:192:ILE:HG13	2.00	0.43
1:K:220:ALA:O	1:K:312:ARG:HD3	2.18	0.43
1:L:105:LEU:O	1:L:134:VAL:HA	2.17	0.43
1:M:359:LYS:HD2	1:M:360:GLN:H	1.83	0.43
1:B:86:TRP:HH2	1:B:119:MET:HG2	1.82	0.43
1:B:9:VAL:HG21	1:B:344:SER:HA	2.00	0.43
1:D:163:VAL:HA	1:D:175:ILE:HG12	2.00	0.43
1:F:73:HIS:HB3	1:F:177:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:22:ALA:HB2	1:J:347:ALA:HB3	1.99	0.43
1:B:119:MET:O	1:B:123:MET:HG2	2.17	0.43
1:D:318:THR:HA	1:D:327:ILE:HD13	1.99	0.43
1:E:41:GLN:HA	1:E:49:GLN:OE1	2.19	0.43
1:H:282:ILE:HG22	1:H:290:ARG:HG2	2.00	0.43
1:K:306:TYR:HA	1:K:307:PRO:HD3	1.86	0.43
1:L:74:GLY:O	1:L:108:ALA:HB2	2.18	0.43
1:N:290:ARG:HH11	1:N:290:ARG:HD3	1.67	0.43
1:D:194:THR:HA	1:D:197:GLY:O	2.18	0.43
1:G:164:PRO:HG3	1:G:174:ALA:HB3	2.01	0.43
1:I:11:ASP:HA	1:I:106:THR:OG1	2.18	0.43
1:L:248:ILE:HG23	1:L:250:ILE:HG12	1.99	0.43
1:K:62:ARG:HG2	1:L:270:GLU:HB2	2.00	0.43
1:L:39:ARG:CZ	1:M:272:ALA:HA	2.48	0.43
1:N:101:HIS:HA	1:N:102:PRO:HD2	1.81	0.43
1:C:238:LYS:HE3	1:C:238:LYS:HA	1.99	0.43
1:I:104:LEU:HG	1:I:133:TYR:HB3	2.00	0.43
1:N:299:MET:HG3	1:N:329:ILE:HG21	2.00	0.43
1:C:170:ALA:O	1:C:172:PRO:HD3	2.19	0.43
1:C:210:ARG:HB3	1:C:210:ARG:CZ	2.48	0.43
1:F:116:ARG:HE	1:F:371:HIS:HA	1.83	0.43
1:G:198:TYR:CZ	1:G:248:ILE:HA	2.54	0.43
1:J:165:ILE:HA	1:J:169:TYR:O	2.19	0.43
1:L:44:MET:HB2	1:L:47:MET:HB2	2.01	0.43
1:B:111:ASN:HA	1:B:112:PRO:HD3	1.83	0.43
1:B:186:THR:HG21	1:B:210:ARG:HG2	2.01	0.43
1:B:210:ARG:O	1:B:213:LYS:HB3	2.19	0.43
1:F:239:SER:HA	1:F:248:ILE:O	2.18	0.43
1:D:57:GLU:HB3	1:F:288:ASP:OD1	2.18	0.43
1:F:306:TYR:HA	1:F:307:PRO:HD3	1.90	0.43
1:G:111:ASN:HA	1:G:112:PRO:HD3	1.86	0.43
1:G:13:GLY:O	1:G:15:GLY:N	2.50	0.43
1:G:193:LEU:O	1:G:198:TYR:HB2	2.18	0.43
1:G:357:ILE:HG21	1:G:370:VAL:HG22	2.00	0.43
1:M:265:SER:HA	1:M:270:GLU:CD	2.39	0.43
1:M:357:ILE:CD1	1:M:373:LYS:HD2	2.48	0.43
1:D:42:GLY:HA2	1:F:171:LEU:HD11	2.01	0.43
1:E:17:VAL:O	1:E:30:VAL:HA	2.18	0.43
1:E:196:ARG:O	1:F:177:ARG:NH2	2.52	0.43
1:D:199:SER:HB3	1:E:75:ILE:HG12	2.00	0.43
1:G:172:PRO:HA	1:G:175:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:203:THR:C	1:J:205:GLU:H	2.23	0.43
1:M:100:GLU:HG3	1:M:101:HIS:HD2	1.82	0.43
1:M:212:ILE:HG23	1:M:216:LEU:HD12	2.01	0.43
1:N:147:ARG:CZ	1:N:330:ILE:HG12	2.48	0.43
1:B:108:ALA:HA	1:B:109:PRO:HD3	1.91	0.43
1:B:290:ARG:HA	1:B:293:LEU:HB2	2.00	0.43
1:D:202:THR:HA	1:E:179:ASP:OD1	2.19	0.43
1:M:58:ALA:HB1	1:M:65:LEU:HD11	2.01	0.43
1:N:151:ILE:O	1:N:297:ASN:HA	2.19	0.43
1:A:61:LYS:O	1:A:63:GLY:HA3	2.19	0.42
1:A:53:TYR:CD1	1:A:65:LEU:HD21	2.54	0.42
1:B:262:PHE:O	1:B:275:HIS:HE1	2.02	0.42
1:C:194:THR:HG22	1:C:198:TYR:O	2.19	0.42
1:D:189:LEU:HD13	1:D:257:CYS:SG	2.59	0.42
1:D:71:ILE:HA	1:D:76:ILE:HA	2.01	0.42
1:F:220:ALA:HB1	1:F:222:ASP:O	2.19	0.42
1:G:104:LEU:HA	1:G:133:TYR:O	2.19	0.42
1:I:99:GLU:HA	1:I:129:VAL:HA	2.01	0.42
1:J:113:LYS:HZ2	1:J:113:LYS:HB3	1.85	0.42
1:K:118:LYS:NZ	1:K:121:GLN:OE1	2.49	0.42
1:K:285:CYS:HB3	1:K:289:ILE:HD11	2.00	0.42
1:M:252:ASN:H	1:M:252:ASN:ND2	2.17	0.42
1:N:269:MET:SD	1:N:269:MET:N	2.92	0.42
1:A:278:THR:HG21	1:A:297:ASN:OD1	2.18	0.42
1:B:136:ILE:HD12	1:B:136:ILE:H	1.83	0.42
1:B:357:ILE:HD13	1:B:373:LYS:HD3	2.01	0.42
1:E:305:MET:HA	1:E:335:ARG:NH1	2.34	0.42
1:G:262:PHE:O	1:G:275:HIS:HE1	2.02	0.42
1:K:195:GLU:HG2	1:L:112:PRO:HG3	2.00	0.42
1:N:113:LYS:O	1:N:116:ARG:HB3	2.19	0.42
1:A:190:MET:HB2	1:A:209:VAL:HG11	2.01	0.42
1:A:217:CYS:SG	1:A:257:CYS:SG	3.15	0.42
1:C:149:THR:HA	1:C:165:ILE:O	2.19	0.42
1:E:10:CYS:HA	1:E:18:LYS:O	2.19	0.42
1:F:45:VAL:CG1	1:H:167:GLU:CG	2.93	0.42
1:K:262:PHE:O	1:K:275:HIS:HE1	2.01	0.42
1:L:163:VAL:HG22	1:L:175:ILE:HG23	2.01	0.42
1:L:283:MET:SD	1:L:290:ARG:NH2	2.92	0.42
1:M:189:LEU:HD13	1:M:257:CYS:SG	2.59	0.42
1:A:36:GLY:CA	1:A:66:THR:O	2.67	0.42
1:B:31:PHE:HA	1:B:32:PRO:HD2	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:ASP:HA	1:G:106:THR:OG1	2.19	0.42
1:J:147:ARG:NH1	1:J:296:ASN:OD1	2.53	0.42
1:A:50:LYS:HD3	1:A:53:TYR:CZ	2.54	0.42
1:G:294:TYR:O	1:G:327:ILE:HA	2.19	0.42
1:J:32:PRO:HB2	1:J:34:ILE:HG12	2.01	0.42
1:J:61:LYS:O	1:J:65:LEU:HG	2.20	0.42
1:M:290:ARG:HA	1:M:293:LEU:HB2	2.01	0.42
1:B:111:ASN:HD21	1:B:115:ASN:ND2	2.18	0.42
1:D:236:LEU:O	1:D:251:GLY:HA2	2.20	0.42
1:D:59:GLN:O	1:D:62:ARG:HD2	2.19	0.42
1:E:147:ARG:NH1	1:E:296:ASN:OD1	2.52	0.42
1:E:180:LEU:HG	1:E:264:PRO:HB3	2.02	0.42
1:I:186:THR:O	1:I:189:LEU:HB3	2.20	0.42
1:K:36:GLY:HA3	1:K:65:LEU:HD13	2.02	0.42
1:L:286:ASP:O	1:L:290:ARG:NH1	2.53	0.42
1:C:154:ASP:O	1:C:160:THR:HA	2.20	0.42
1:B:60:SER:C	1:D:287:ILE:HG21	2.40	0.42
1:E:313:MET:O	1:E:317:ILE:HG12	2.20	0.42
1:J:217:CYS:HA	1:J:254:ARG:O	2.20	0.42
1:L:103:THR:H	1:L:132:MET:HA	1.84	0.42
1:M:10:CYS:HA	1:M:18:LYS:O	2.20	0.42
1:N:163:VAL:HG22	1:N:175:ILE:HG23	2.02	0.42
1:A:11:ASP:HA	1:A:106:THR:OG1	2.19	0.42
1:A:161:HIS:HA	1:A:176:MET:O	2.19	0.42
1:B:11:ASP:HA	1:B:106:THR:OG1	2.19	0.42
1:D:164:PRO:HG2	1:D:171:LEU:HB3	2.02	0.42
1:E:197:GLY:HA2	1:F:177:ARG:NH1	2.34	0.42
1:E:306:TYR:HA	1:E:307:PRO:HD3	1.92	0.42
1:D:46:GLY:O	1:F:167:GLU:OE2	2.38	0.42
1:F:219:VAL:HG22	1:F:258:PRO:HB3	2.02	0.42
1:F:45:VAL:CG2	1:H:166:TYR:HD1	2.16	0.42
1:G:11:ASP:HB3	1:G:18:LYS:HD2	2.01	0.42
1:H:204:ALA:HB3	1:J:287:ILE:HB	2.01	0.42
1:I:142:LEU:HD22	1:I:165:ILE:HB	2.02	0.42
1:J:9:VAL:HA	1:J:104:LEU:O	2.20	0.42
1:J:328:LYS:HB3	1:J:328:LYS:HE3	1.83	0.42
1:N:304:THR:O	1:N:309:ILE:HG21	2.19	0.42
1:A:102:PRO:HA	1:A:131:ALA:O	2.19	0.42
1:A:305:MET:HA	1:A:335:ARG:NH1	2.35	0.42
1:B:134:VAL:O	1:B:374:CYS:SG	2.78	0.42
1:B:162:ASN:OD1	1:B:277:THR:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:HIS:O	1:C:130:PRO:HD2	2.20	0.42
1:F:102:PRO:HA	1:F:131:ALA:O	2.20	0.42
1:F:289:ILE:O	1:F:291:LYS:HD3	2.20	0.42
1:D:44:MET:SD	1:F:293:LEU:HD22	2.52	0.42
1:H:135:ALA:HB3	1:H:140:LEU:HD11	2.02	0.42
1:L:138:ALA:HB2	1:L:163:VAL:HG21	2.02	0.42
1:A:39:ARG:NH1	1:B:267:ILE:HG22	2.34	0.42
1:D:43:VAL:HG22	1:F:171:LEU:CB	2.50	0.42
1:I:187:ASP:O	1:I:190:MET:HB3	2.20	0.42
1:I:213:LYS:HA	1:I:217:CYS:SG	2.59	0.42
1:K:299:MET:HB3	1:K:304:THR:HG21	2.00	0.42
1:L:86:TRP:CH2	1:L:119:MET:HG3	2.55	0.42
1:N:11:ASP:HA	1:N:106:THR:OG1	2.19	0.42
1:A:162:ASN:O	1:A:175:ILE:HA	2.19	0.41
1:B:290:ARG:HA	1:B:293:LEU:HD12	2.02	0.41
1:C:70:PRO:HB3	1:C:81:ASP:HB2	2.02	0.41
1:D:61:LYS:HZ1	1:F:291:LYS:CG	2.32	0.41
1:F:318:THR:HA	1:F:327:ILE:HD13	2.02	0.41
1:J:304:THR:O	1:J:309:ILE:HG21	2.19	0.41
1:K:230:ALA:HB1	1:K:252:ASN:HD22	1.84	0.41
1:N:328:LYS:HZ1	1:N:330:ILE:HG13	1.85	0.41
1:A:36:GLY:O	1:A:52:SER:HA	2.20	0.41
1:A:98:PRO:HG2	1:A:128:ASN:HD21	1.85	0.41
1:C:213:LYS:O	1:C:217:CYS:HB2	2.20	0.41
1:F:8:LEU:HG	1:F:101:HIS:HB3	2.02	0.41
1:F:99:GLU:CD	1:F:99:GLU:H	2.23	0.41
1:G:153:LEU:HD21	1:G:274:ILE:HD12	2.02	0.41
1:I:285:CYS:HB3	1:I:289:ILE:HD11	2.01	0.41
1:J:107:GLU:OE1	1:J:112:PRO:HG3	2.21	0.41
1:K:264:PRO:HD2	1:K:271:SER:O	2.20	0.41
1:N:153:LEU:HD21	1:N:274:ILE:HG23	2.02	0.41
1:D:189:LEU:HD12	1:D:192:ILE:HD11	2.02	0.41
1:D:196:ARG:HA	1:E:113:LYS:HD2	2.02	0.41
1:G:4:GLU:HG2	1:G:5:THR:HG23	2.02	0.41
1:I:11:ASP:OD1	1:I:18:LYS:NZ	2.51	0.41
1:I:171:LEU:HA	1:I:172:PRO:HD2	1.93	0.41
1:M:186:THR:OG1	1:M:213:LYS:HD2	2.19	0.41
1:N:322:PRO:O	1:N:327:ILE:HD11	2.20	0.41
1:D:17:VAL:O	1:D:30:VAL:HA	2.21	0.41
1:D:45:VAL:HG11	1:F:165:ILE:CD1	2.47	0.41
1:E:174:ALA:HA	1:E:284:LYS:HZ3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:ILE:HG22	1:F:313:MET:SD	2.60	0.41
1:G:39:ARG:HD3	1:G:66:THR:HG23	2.01	0.41
1:J:306:TYR:HA	1:J:307:PRO:HD3	1.96	0.41
1:L:242:LEU:H	1:L:245:GLY:HA3	1.84	0.41
1:F:160:THR:O	1:F:177:ARG:HA	2.21	0.41
1:H:180:LEU:HD11	1:H:264:PRO:HB3	2.03	0.41
1:I:264:PRO:HB2	1:I:271:SER:HB3	2.03	0.41
1:J:10:CYS:HA	1:J:19:ALA:HA	2.01	0.41
1:B:116:ARG:HH12	1:B:375:PHE:HD2	1.68	0.41
1:B:9:VAL:O	1:B:19:ALA:HA	2.20	0.41
1:C:34:ILE:O	1:C:54:VAL:HA	2.21	0.41
1:D:190:MET:HB2	1:D:209:VAL:HG11	2.03	0.41
1:F:11:ASP:OD1	1:F:18:LYS:NZ	2.51	0.41
1:F:269:MET:O	1:F:270:GLU:HB2	2.21	0.41
1:H:163:VAL:HA	1:H:175:ILE:HG12	2.02	0.41
1:H:239:SER:HA	1:H:248:ILE:O	2.21	0.41
1:K:98:PRO:O	1:K:129:VAL:HA	2.21	0.41
1:L:253:GLU:HG3	1:L:256:ARG:HH21	1.85	0.41
1:M:160:THR:OG1	1:M:181:ALA:HB2	2.20	0.41
1:N:274:ILE:HG22	1:N:313:MET:SD	2.61	0.41
1:N:362:TYR:OH	1:N:367:PRO:HG3	2.21	0.41
1:N:71:ILE:HG23	1:N:76:ILE:HG12	2.01	0.41
1:A:38:PRO:HB2	1:A:40:HIS:O	2.21	0.41
1:B:113:LYS:O	1:B:116:ARG:HB3	2.21	0.41
1:B:203:THR:HG21	1:C:268:GLY:O	2.20	0.41
1:D:10:CYS:HA	1:D:18:LYS:O	2.20	0.41
1:E:190:MET:CA	1:E:209:VAL:HG11	2.51	0.41
1:F:11:ASP:O	1:F:17:VAL:HA	2.21	0.41
1:E:62:ARG:NH2	1:F:266:PHE:O	2.52	0.41
1:H:101:HIS:O	1:H:130:PRO:HD2	2.20	0.41
1:J:152:VAL:O	1:J:162:ASN:HA	2.19	0.41
1:K:190:MET:HA	1:K:209:VAL:HG11	2.02	0.41
1:A:200:PHE:HA	1:A:205:GLU:HB3	2.03	0.41
1:A:61:LYS:C	1:A:63:GLY:HA3	2.41	0.41
1:B:10:CYS:HB3	1:B:105:LEU:HD23	2.01	0.41
1:B:8:LEU:HG	1:B:101:HIS:HB3	2.03	0.41
1:B:63:GLY:C	1:C:267:ILE:HA	2.40	0.41
1:E:101:HIS:HA	1:E:102:PRO:HD2	1.96	0.41
1:N:113:LYS:HB2	1:N:113:LYS:HE3	1.94	0.41
1:F:213:LYS:HD3	1:F:214:GLU:HG3	2.02	0.41
1:G:287:ILE:HA	1:G:290:ARG:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:17:VAL:O	1:G:30:VAL:HA	2.20	0.41
1:H:189:LEU:HD12	1:H:192:ILE:HD11	2.03	0.41
1:I:201:VAL:HG21	1:J:179:ASP:OD2	2.21	0.41
1:M:359:LYS:HD2	1:M:360:GLN:HB2	2.02	0.41
1:N:304:THR:HA	1:N:309:ILE:HD13	2.02	0.41
1:B:289:ILE:HA	1:B:292:ASP:OD2	2.21	0.41
1:E:162:ASN:OD1	1:E:277:THR:HG23	2.21	0.41
1:E:191:LYS:HD2	1:F:176:MET:HG2	2.02	0.41
1:G:196:ARG:HE	1:G:249:THR:HG23	1.86	0.41
1:H:149:THR:HA	1:H:165:ILE:O	2.21	0.41
1:J:202:THR:HG21	1:L:285:CYS:HA	2.03	0.41
1:A:186:THR:O	1:A:189:LEU:HB3	2.21	0.41
1:A:281:SER:HA	1:A:284:LYS:NZ	2.36	0.41
1:C:101:HIS:HA	1:C:102:PRO:HD2	1.86	0.41
1:C:305:MET:SD	1:C:336:LYS:HB3	2.61	0.41
1:E:162:ASN:O	1:E:175:ILE:HA	2.20	0.41
1:E:218:TYR:O	1:E:255:PHE:HA	2.21	0.41
1:E:219:VAL:HG22	1:E:258:PRO:CB	2.51	0.41
1:D:39:ARG:NH2	1:E:271:SER:O	2.54	0.41
1:G:159:VAL:HA	1:G:178:LEU:O	2.20	0.41
1:F:46:GLY:N	1:H:167:GLU:HB3	2.32	0.41
1:I:17:VAL:O	1:I:30:VAL:HA	2.21	0.41
1:N:118:LYS:NZ	1:N:121:GLN:OE1	2.48	0.41
1:A:188:TYR:CE2	1:A:257:CYS:HA	2.56	0.40
1:C:304:THR:HA	1:C:309:ILE:HD13	2.03	0.40
1:D:359:LYS:NZ	1:D:360:GLN:OE1	2.54	0.40
1:D:45:VAL:CA	1:F:165:ILE:H	2.34	0.40
1:F:108:ALA:O	1:F:111:ASN:HB2	2.21	0.40
1:G:38:PRO:HD2	1:G:51:ASP:O	2.21	0.40
1:I:9:VAL:O	1:I:19:ALA:HA	2.22	0.40
1:I:210:ARG:O	1:I:213:LYS:HB3	2.21	0.40
1:J:248:ILE:HA	1:J:248:ILE:HD12	1.97	0.40
1:K:155:SER:HA	1:K:160:THR:HA	2.03	0.40
1:L:34:ILE:O	1:L:54:VAL:HA	2.22	0.40
1:M:291:LYS:HG3	1:M:292:ASP:H	1.85	0.40
1:N:294:TYR:O	1:N:327:ILE:HA	2.21	0.40
1:A:112:PRO:O	1:A:115:ASN:HB3	2.21	0.40
1:A:137:GLN:HG2	1:A:339:VAL:CG1	2.48	0.40
1:B:32:PRO:HB2	1:B:34:ILE:HG12	2.03	0.40
1:D:217:CYS:HA	1:D:254:ARG:O	2.21	0.40
1:D:9:VAL:O	1:D:19:ALA:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:108:ALA:O	1:J:111:ASN:HB2	2.22	0.40
1:M:53:TYR:HB2	1:N:268:GLY:HA2	2.03	0.40
1:N:14:SER:O	1:N:183:ARG:NH2	2.53	0.40
1:N:79:TRP:HA	1:N:82:MET:HB2	2.02	0.40
1:A:99:GLU:CD	1:A:99:GLU:H	2.25	0.40
1:B:190:MET:HA	1:B:209:VAL:HG11	2.04	0.40
1:A:44:MET:SD	1:C:166:TYR:HD1	2.45	0.40
1:C:8:LEU:HA	1:C:20:GLY:O	2.22	0.40
1:E:11:ASP:OD1	1:E:18:LYS:NZ	2.52	0.40
1:F:100:GLU:HG3	1:F:101:HIS:CD2	2.55	0.40
1:I:11:ASP:HB3	1:I:18:LYS:HB2	2.03	0.40
1:M:10:CYS:HB3	1:M:105:LEU:HD23	2.04	0.40
1:M:328:LYS:HZ1	1:M:330:ILE:HG12	1.86	0.40
1:E:161:HIS:HA	1:E:176:MET:O	2.20	0.40
1:I:155:SER:HB3	1:I:304:THR:HG23	2.03	0.40
1:L:50:LYS:NZ	1:L:52:SER:O	2.51	0.40
1:M:33:SER:O	1:M:34:ILE:HG23	2.22	0.40
1:C:243:PRO:O	1:E:291:LYS:HB3	2.21	0.40
1:D:202:THR:N	1:D:205:GLU:HB2	2.37	0.40
1:D:198:TYR:CE2	1:D:248:ILE:HG23	2.57	0.40
1:F:101:HIS:HA	1:F:102:PRO:HD2	1.85	0.40
1:D:46:GLY:HA2	1:F:149:THR:HA	2.04	0.40
1:H:10:CYS:HA	1:H:18:LYS:O	2.22	0.40
1:H:19:ALA:HB3	1:H:29:ALA:HB3	2.04	0.40
1:H:31:PHE:HA	1:H:32:PRO:HD2	1.92	0.40
1:I:132:MET:HG3	1:I:357:ILE:HB	2.03	0.40
1:K:151:ILE:O	1:K:297:ASN:HA	2.22	0.40
1:K:171:LEU:O	1:K:175:ILE:HG13	2.22	0.40
1:K:332:PRO:HB2	1:K:335:ARG:HB3	2.03	0.40
1:L:193:LEU:HD21	1:L:212:ILE:HD13	2.03	0.40
1:L:38:PRO:HD2	1:L:51:ASP:O	2.21	0.40
1:M:279:TYR:O	1:M:283:MET:HB2	2.21	0.40
1:M:75:ILE:HG23	1:M:111:ASN:ND2	2.36	0.40

There are no symmetry-related clashes.



## 4.3 Torsion angles

### 4.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	373/377 (99%)	297 (80%)	63 (17%)	13 (4%)	4	32
1	B	373/377 (99%)	298 (80%)	58 (16%)	17 (5%)	2	27
1	C	373/377 (99%)	310 (83%)	55 (15%)	8 (2%)	8	43
1	D	373/377 (99%)	310 (83%)	49 (13%)	14 (4%)	3	30
1	E	373/377 (99%)	303 (81%)	56 (15%)	14 (4%)	3	30
1	F	373/377 (99%)	291 (78%)	62 (17%)	20 (5%)	2	24
1	G	373/377 (99%)	315 (84%)	46 (12%)	12 (3%)	4	34
1	H	373/377 (99%)	308 (83%)	55 (15%)	10 (3%)	5	38
1	I	373/377 (99%)	318 (85%)	45 (12%)	10 (3%)	5	38
1	J	373/377 (99%)	308 (83%)	48 (13%)	17 (5%)	2	27
1	K	373/377 (99%)	323 (87%)	33 (9%)	17 (5%)	2	27
1	L	373/377 (99%)	311 (83%)	44 (12%)	18 (5%)	2	26
1	M	373/377 (99%)	300 (80%)	54 (14%)	19 (5%)	2	25
1	N	373/377 (99%)	307 (82%)	51 (14%)	15 (4%)	3	29
All	All	5222/5278 (99%)	4299 (82%)	719 (14%)	204 (4%)	3	30

All (204) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	236	LEU
1	A	252	ASN
1	A	272	ALA
1	B	113	LYS
1	B	323	SER
1	C	236	LEU
1	D	49	GLN
1	D	61	LYS

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Mol	Chain	Res	Type
1	D	236	LEU
1	D	323	SER
1	E	111	ASN
1	E	128	ASN
1	E	222	ASP
1	E	263	GLN
1	E	266	PHE
1	E	359	LYS
1	F	14	SER
1	F	173	HIS
1	F	254	ARG
1	F	265	SER
1	F	270	GLU
1	F	282	ILE
1	F	289	ILE
1	G	14	SER
1	G	222	ASP
1	H	62	ARG
1	H	236	LEU
1	I	236	LEU
1	J	112	PRO
1	J	137	GLN
1	J	175	ILE
1	J	242	LEU
1	J	335	ARG
1	K	234	SER
1	K	267	ILE
1	K	270	GLU
1	K	350	SER
1	L	236	LEU
1	L	325	MET
1	M	2	GLU
1	M	37	ARG
1	M	173	HIS
1	M	236	LEU
1	M	263	GLN
1	N	47	MET
1	N	322	PRO
1	A	55	GLY
1	A	61	LYS
1	A	181	ALA
1	B	2	GLU

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Mol	Chain	Res	Type
1	B	4	GLU
1	B	14	SER
1	B	45	VAL
1	B	199	SER
1	B	252	ASN
1	B	254	ARG
1	C	181	ALA
1	D	69	TYR
1	D	113	LYS
1	D	267	ILE
1	D	335	ARG
1	E	14	SER
1	F	4	GLU
1	F	266	PHE
1	F	290	ARG
1	G	113	LYS
1	G	236	LEU
1	H	2	GLU
1	H	323	SER
1	I	253	GLU
1	J	14	SER
1	J	359	LYS
1	K	266	PHE
1	K	323	SER
1	K	335	ARG
1	L	62	ARG
1	L	204	ALA
1	L	291	LYS
1	L	359	LYS
1	M	41	GLN
1	M	67	LEU
1	M	68	LYS
1	M	323	SER
1	M	359	LYS
1	N	14	SER
1	N	128	ASN
1	N	267	ILE
1	A	2	GLU
1	A	335	ARG
1	A	374	CYS
1	B	181	ALA
1	C	204	ALA

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Mol	Chain	Res	Type
1	D	15	GLY
1	D	60	SER
1	E	73	HIS
1	E	157	ASP
1	F	44	MET
1	F	222	ASP
1	F	234	SER
1	F	359	LYS
1	G	359	LYS
1	H	181	ALA
1	H	359	LYS
1	I	2	GLU
1	I	335	ARG
1	J	272	ALA
1	K	181	ALA
1	K	236	LEU
1	K	359	LYS
1	L	2	GLU
1	L	49	GLN
1	L	112	PRO
1	L	222	ASP
1	L	254	ARG
1	L	286	ASP
1	M	270	GLU
1	M	283	MET
1	M	335	ARG
1	N	2	GLU
1	N	62	ARG
1	N	175	ILE
1	B	359	LYS
1	D	359	LYS
1	E	335	ARG
1	F	283	MET
1	F	285	CYS
1	G	2	GLU
1	G	4	GLU
1	G	181	ALA
1	G	242	LEU
1	H	14	SER
1	H	335	ARG
1	H	374	CYS
1	I	222	ASP

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Mol	Chain	Res	Type
1	J	234	SER
1	J	274	ILE
1	K	63	GLY
1	K	222	ASP
1	K	233	SER
1	K	243	PRO
1	L	15	GLY
1	L	181	ALA
1	L	246	GLN
1	M	242	LEU
1	N	181	ALA
1	N	222	ASP
1	N	251	GLY
1	N	270	GLU
1	A	222	ASP
1	B	234	SER
1	B	274	ILE
1	B	373	LYS
1	C	14	SER
1	C	274	ILE
1	C	335	ARG
1	D	253	GLU
1	E	62	ARG
1	F	264	PRO
1	G	253	GLU
1	H	274	ILE
1	I	14	SER
1	J	15	GLY
1	J	171	LEU
1	J	244	ASP
1	K	251	GLY
1	L	263	GLN
1	M	38	PRO
1	M	181	ALA
1	N	234	SER
1	A	372	ARG
1	B	222	ASP
1	C	62	ARG
1	D	181	ALA
1	E	171	LEU
1	F	109	PRO
1	F	251	GLY

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Mol	Chain	Res	Type
1	I	181	ALA
1	I	242	LEU
1	J	136	ILE
1	J	374	CYS
1	K	274	ILE
1	M	159	VAL
1	M	171	LEU
1	B	339	VAL
1	E	15	GLY
1	K	175	ILE
1	L	251	GLY
1	A	242	LEU
1	D	175	ILE
1	F	274	ILE
1	I	159	VAL
1	L	243	PRO
1	M	175	ILE
1	G	251	GLY
1	I	251	GLY
1	J	111	ASN
1	B	159	VAL
1	C	175	ILE
1	G	274	ILE
1	J	71	ILE
1	N	43	VAL
1	N	159	VAL
1	E	267	ILE

#### 4.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	318/320 (99%)	284 (89%)	34 (11%)	7	28
1	B	318/320 (99%)	285 (90%)	33 (10%)	8	29
1	C	318/320 (99%)	281 (88%)	37 (12%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	318/320 (99%)	284 (89%)	34 (11%)	7	28
1	E	318/320 (99%)	282 (89%)	36 (11%)	6	26
1	F	318/320 (99%)	287 (90%)	31 (10%)	9	32
1	G	318/320 (99%)	294 (92%)	24 (8%)	15	45
1	H	318/320 (99%)	291 (92%)	27 (8%)	12	40
1	I	318/320 (99%)	288 (91%)	30 (9%)	9	33
1	J	318/320 (99%)	277 (87%)	41 (13%)	5	22
1	K	318/320 (99%)	289 (91%)	29 (9%)	10	35
1	L	318/320 (99%)	286 (90%)	32 (10%)	8	30
1	M	318/320 (99%)	286 (90%)	32 (10%)	8	30
1	N	318/320 (99%)	271 (85%)	47 (15%)	3	18
All	All	4452/4480 (99%)	3985 (90%)	467 (10%)	7	29

All (467) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	18	LYS
1	A	61	LYS
1	A	66	THR
1	A	99	GLU
1	A	109	PRO
1	A	112	PRO
1	A	115	ASN
1	A	128	ASN
1	A	159	VAL
1	A	176	MET
1	A	195	GLU
1	A	207	GLU
1	A	210	ARG
1	A	215	LYS
1	A	218	TYR
1	A	221	LEU
1	A	238	LYS
1	A	244	ASP
1	A	249	THR
1	A	252	ASN
1	A	263	GLN

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Mol	Chain	Res	Type
1	A	266	PHE
1	A	270	GLU
1	A	275	HIS
1	A	277	THR
1	A	287	ILE
1	A	288	ASP
1	A	292	ASP
1	A	297	ASN
1	A	303	THR
1	A	316	GLU
1	A	334	GLU
1	A	359	LYS
1	B	18	LYS
1	B	62	ARG
1	B	66	THR
1	B	100	GLU
1	B	107	GLU
1	B	115	ASN
1	B	128	ASN
1	B	155	SER
1	B	159	VAL
1	B	166	TYR
1	B	169	TYR
1	B	187	ASP
1	B	195	GLU
1	B	207	GLU
1	B	213	LYS
1	B	218	TYR
1	B	221	LEU
1	B	238	LYS
1	B	249	THR
1	B	252	ASN
1	B	263	GLN
1	B	284	LYS
1	B	285	CYS
1	B	288	ASP
1	B	293	LEU
1	B	297	ASN
1	B	303	THR
1	B	311	ASP
1	B	316	GLU
1	B	324	THR

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Mol	Chain	Res	Type
1	B	334	GLU
1	B	356	TRP
1	B	359	LYS
1	C	2	GLU
1	C	18	LYS
1	C	51	ASP
1	C	77	THR
1	C	100	GLU
1	C	109	PRO
1	C	115	ASN
1	C	126	THR
1	C	128	ASN
1	C	155	SER
1	C	159	VAL
1	C	167	GLU
1	C	172	PRO
1	C	173	HIS
1	C	176	MET
1	C	180	LEU
1	C	207	GLU
1	C	213	LYS
1	C	218	TYR
1	C	221	LEU
1	C	238	LYS
1	C	244	ASP
1	C	249	THR
1	C	252	ASN
1	C	256	ARG
1	C	263	GLN
1	C	265	SER
1	C	277	THR
1	C	278	THR
1	C	284	LYS
1	C	287	ILE
1	C	291	LYS
1	C	292	ASP
1	C	297	ASN
1	C	334	GLU
1	C	348	SER
1	C	359	LYS
1	D	16	LEU
1	D	18	LYS

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Mol	Chain	Res	Type
1	D	44	MET
1	D	45	VAL
1	D	53	TYR
1	D	59	GLN
1	D	62	ARG
1	D	66	THR
1	D	77	THR
1	D	99	GLU
1	D	103	THR
1	D	109	PRO
1	D	128	ASN
1	D	159	VAL
1	D	176	MET
1	D	201	VAL
1	D	207	GLU
1	D	221	LEU
1	D	224	GLU
1	D	226	GLU
1	D	238	LYS
1	D	252	ASN
1	D	263	GLN
1	D	266	PHE
1	D	277	THR
1	D	284	LYS
1	D	292	ASP
1	D	297	ASN
1	D	311	ASP
1	D	316	GLU
1	D	334	GLU
1	D	356	TRP
1	D	359	LYS
1	D	371	HIS
1	E	14	SER
1	E	18	LYS
1	E	49	GLN
1	E	51	ASP
1	E	56	ASP
1	E	57	GLU
1	E	67	LEU
1	E	80	ASP
1	E	109	PRO
1	E	115	ASN

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Mol	Chain	Res	Type
1	E	128	ASN
1	E	157	ASP
1	E	176	MET
1	E	180	LEU
1	E	187	ASP
1	E	188	TYR
1	E	190	MET
1	E	195	GLU
1	E	209	VAL
1	E	213	LYS
1	E	226	GLU
1	E	238	LYS
1	E	249	THR
1	E	267	ILE
1	E	269	MET
1	E	277	THR
1	E	284	LYS
1	E	286	ASP
1	E	288	ASP
1	E	292	ASP
1	E	297	ASN
1	E	316	GLU
1	E	334	GLU
1	E	352	PHE
1	E	357	ILE
1	E	359	LYS
1	F	18	LYS
1	F	99	GLU
1	F	115	ASN
1	F	121	GLN
1	F	128	ASN
1	F	149	THR
1	F	162	ASN
1	F	166	TYR
1	F	171	LEU
1	F	180	LEU
1	F	187	ASP
1	F	199	SER
1	F	203	THR
1	F	207	GLU
1	F	213	LYS
1	F	221	LEU

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Mol	Chain	Res	Type
1	F	238	LYS
1	F	248	ILE
1	F	249	THR
1	F	263	GLN
1	F	270	GLU
1	F	277	THR
1	F	288	ASP
1	F	291	LYS
1	F	292	ASP
1	F	297	ASN
1	F	303	THR
1	F	311	ASP
1	F	334	GLU
1	F	352	PHE
1	F	359	LYS
1	G	18	LYS
1	G	51	ASP
1	G	62	ARG
1	G	66	THR
1	G	99	GLU
1	G	128	ASN
1	G	159	VAL
1	G	176	MET
1	G	203	THR
1	G	213	LYS
1	G	218	TYR
1	G	238	LYS
1	G	252	ASN
1	G	263	GLN
1	G	264	PRO
1	G	276	GLU
1	G	293	LEU
1	G	297	ASN
1	G	303	THR
1	G	311	ASP
1	G	334	GLU
1	G	359	LYS
1	G	368	SER
1	G	372	ARG
1	H	2	GLU
1	H	18	LYS
1	H	99	GLU

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Mol	Chain	Res	Type
1	H	109	PRO
1	H	128	ASN
1	H	159	VAL
1	H	176	MET
1	H	207	GLU
1	H	210	ARG
1	H	215	LYS
1	H	218	TYR
1	H	221	LEU
1	H	238	LYS
1	H	244	ASP
1	H	248	ILE
1	H	249	THR
1	H	252	ASN
1	H	260	THR
1	H	263	GLN
1	H	277	THR
1	H	284	LYS
1	H	297	ASN
1	H	334	GLU
1	H	356	TRP
1	H	359	LYS
1	H	368	SER
1	H	371	HIS
1	I	2	GLU
1	I	18	LYS
1	I	49	GLN
1	I	57	GLU
1	I	59	GLN
1	I	62	ARG
1	I	100	GLU
1	I	109	PRO
1	I	128	ASN
1	I	159	VAL
1	I	176	MET
1	I	187	ASP
1	I	207	GLU
1	I	210	ARG
1	I	218	TYR
1	I	221	LEU
1	I	238	LYS
1	I	248	ILE

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Mol	Chain	Res	Type
1	I	252	ASN
1	I	253	GLU
1	I	260	THR
1	I	263	GLN
1	I	284	LYS
1	I	297	ASN
1	I	303	THR
1	I	334	GLU
1	I	356	TRP
1	I	359	LYS
1	I	368	SER
1	I	371	HIS
1	J	2	GLU
1	J	18	LYS
1	J	62	ARG
1	J	75	ILE
1	J	80	ASP
1	J	100	GLU
1	J	111	ASN
1	J	112	PRO
1	J	115	ASN
1	J	128	ASN
1	J	134	VAL
1	J	159	VAL
1	J	179	ASP
1	J	194	THR
1	J	199	SER
1	J	201	VAL
1	J	202	THR
1	J	207	GLU
1	J	208	ILE
1	J	213	LYS
1	J	218	TYR
1	J	221	LEU
1	J	238	LYS
1	J	242	LEU
1	J	246	GLN
1	J	252	ASN
1	J	257	CYS
1	J	263	GLN
1	J	266	PHE
1	J	267	ILE

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Mol	Chain	Res	Type
1	J	277	THR
1	J	284	LYS
1	J	286	ASP
1	J	292	ASP
1	J	297	ASN
1	J	311	ASP
1	J	323	SER
1	J	334	GLU
1	J	348	SER
1	J	359	LYS
1	J	368	SER
1	K	4	GLU
1	K	18	LYS
1	K	62	ARG
1	K	99	GLU
1	K	128	ASN
1	K	159	VAL
1	K	173	HIS
1	K	176	MET
1	K	187	ASP
1	K	195	GLU
1	K	203	THR
1	K	207	GLU
1	K	213	LYS
1	K	215	LYS
1	K	221	LEU
1	K	238	LYS
1	K	242	LEU
1	K	244	ASP
1	K	252	ASN
1	K	257	CYS
1	K	263	GLN
1	K	277	THR
1	K	286	ASP
1	K	297	ASN
1	K	311	ASP
1	K	334	GLU
1	K	357	ILE
1	K	359	LYS
1	K	371	HIS
1	L	2	GLU
1	L	3	ASP

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Mol	Chain	Res	Type
1	L	4	GLU
1	L	18	LYS
1	L	51	ASP
1	L	72	GLU
1	L	75	ILE
1	L	80	ASP
1	L	99	GLU
1	L	109	PRO
1	L	128	ASN
1	L	132	MET
1	L	148	THR
1	L	159	VAL
1	L	199	SER
1	L	207	GLU
1	L	218	TYR
1	L	221	LEU
1	L	238	LYS
1	L	244	ASP
1	L	252	ASN
1	L	260	THR
1	L	263	GLN
1	L	284	LYS
1	L	289	ILE
1	L	297	ASN
1	L	316	GLU
1	L	326	LYS
1	L	334	GLU
1	L	348	SER
1	L	351	THR
1	L	359	LYS
1	M	2	GLU
1	M	18	LYS
1	M	34	ILE
1	M	38	PRO
1	M	45	VAL
1	M	57	GLU
1	M	62	ARG
1	M	65	LEU
1	M	72	GLU
1	M	77	THR
1	M	103	THR
1	M	128	ASN

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Mol	Chain	Res	Type
1	M	148	THR
1	M	159	VAL
1	M	215	LYS
1	M	218	TYR
1	M	238	LYS
1	M	244	ASP
1	M	248	ILE
1	M	249	THR
1	M	252	ASN
1	M	276	GLU
1	M	277	THR
1	M	284	LYS
1	M	292	ASP
1	M	297	ASN
1	M	303	THR
1	M	324	THR
1	M	334	GLU
1	M	352	PHE
1	M	359	LYS
1	M	368	SER
1	N	2	GLU
1	N	4	GLU
1	N	14	SER
1	N	18	LYS
1	N	24	ASP
1	N	40	HIS
1	N	43	VAL
1	N	44	MET
1	N	51	ASP
1	N	59	GLN
1	N	62	ARG
1	N	100	GLU
1	N	109	PRO
1	N	128	ASN
1	N	132	MET
1	N	148	THR
1	N	159	VAL
1	N	176	MET
1	N	180	LEU
1	N	193	LEU
1	N	199	SER
1	N	210	ARG

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Mol	Chain	Res	Type
1	N	215	LYS
1	N	218	TYR
1	N	221	LEU
1	N	238	LYS
1	N	250	ILE
1	N	252	ASN
1	N	257	CYS
1	N	263	GLN
1	N	266	PHE
1	N	269	MET
1	N	271	SER
1	N	277	THR
1	N	278	THR
1	N	284	LYS
1	N	287	ILE
1	N	297	ASN
1	N	311	ASP
1	N	322	PRO
1	N	324	THR
1	N	325	MET
1	N	326	LYS
1	N	334	GLU
1	N	352	PHE
1	N	359	LYS
1	N	368	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	111	ASN
1	A	115	ASN
1	A	128	ASN
1	A	280	ASN
1	B	41	GLN
1	B	115	ASN
1	B	162	ASN
1	B	263	GLN
1	B	275	HIS
1	D	41	GLN
1	D	111	ASN
1	D	115	ASN

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Mol	Chain	Res	Type
1	D	263	GLN
1	D	275	HIS
1	E	92	ASN
1	E	128	ASN
1	E	252	ASN
1	E	371	HIS
1	F	111	ASN
1	F	115	ASN
1	F	252	ASN
1	F	263	GLN
1	F	280	ASN
1	G	111	ASN
1	G	115	ASN
1	G	162	ASN
1	G	263	GLN
1	G	275	HIS
1	H	111	ASN
1	H	115	ASN
1	H	173	HIS
1	H	263	GLN
1	H	280	ASN
1	I	162	ASN
1	I	263	GLN
1	J	263	GLN
1	K	263	GLN
1	L	92	ASN
1	L	162	ASN
1	L	371	HIS
1	M	111	ASN
1	M	115	ASN
1	M	161	HIS
1	M	246	GLN
1	M	252	ASN
1	N	111	ASN
1	N	115	ASN
1	N	252	ASN

#### 4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

#### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

#### 4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

#### 4.6 Ligand geometry [i](#)

There are no ligands in this entry.

#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.